

# NON-SELF-ADJOINT OPERATORS, INFINITE DETERMINANTS, AND SOME APPLICATIONS

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*With great respect and deep admiration, we dedicate this paper  
to the memory of Boris M. Levitan 1914–2004.*

**ABSTRACT.** We study various spectral theoretic aspects of non-self-adjoint operators. Specifically, we consider a class of factorable non-self-adjoint perturbations of a given unperturbed non-self-adjoint operator and provide an in-depth study of a variant of the Birman–Schwinger principle as well as local and global Weinstein–Aronszajn formulas.

Our applications include a study of suitably symmetrized (modified) perturbation determinants of Schrödinger operators in dimensions  $n = 1, 2, 3$  and their connection with Krein’s spectral shift function in two- and three-dimensional scattering theory. Moreover, we study an appropriate multi-dimensional analog of the celebrated formula by Jost and Pais that identifies Jost functions with suitable Fredholm (perturbation) determinants and hence reduces the latter to simple Wronski determinants.

## 1. INTRODUCTION

This paper has been written in response to the increased demand of spectral theoretic aspects of non-self-adjoint operators in contemporary applied and mathematical physics. What we have in mind, in particular, concerns the following typical two scenarios: First, the construction of certain classes of solutions of a number of completely integrable hierarchies of evolution equations by means of the inverse scattering method, for instance, in the context of the focusing nonlinear Schrödinger equation in  $(1 + 1)$ -dimensions, naturally leads to non-self-adjoint Lax operators. Specifically, in the particular case of the focusing nonlinear Schrödinger equation the corresponding Lax operator is a non-self-adjoint one-dimensional Dirac-type operator. Second, linearizations of nonlinear partial differential equations around steady state and solitary-type solutions, frequently, lead to a linear non-self-adjoint spectral problem. In the latter context, the use of the so-called Evans function (an analog of the one-dimensional Jost function for Schrödinger operators) in the course of a linear stability analysis has become a cornerstone of this circle of ideas. As shown in [15], the Evans function equals a (modified) Fredholm determinant

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associated with an underlying Birman–Schwinger-type operator. This observation naturally leads to the second main theme of this paper and a concrete application to non-self-adjoint operators, viz., a study of properly symmetrized (modified) perturbation determinants of non-self-adjoint Schrödinger operators in dimensions  $n = 1, 2, 3$ .

Next, we briefly summarize the content of each section. In Section 2, following the seminal work of Kato [24] (see also Konno and Kuroda [28] and Howland [20]), we consider a class of factorable non-self-adjoint perturbations, formally given by  $B^*A$ , of a given unperturbed non-self-adjoint operator  $H_0$  in a Hilbert space  $\mathcal{H}$  and introduce a densely defined, closed linear operator  $H$  in  $\mathcal{H}$  which represents an extension of  $H_0 + B^*A$ . Closely following Konno and Kuroda [28], we subsequently derive a general Birman–Schwinger principle for  $H$  in Section 3. A variant of the essential spectrum of  $H$  and a local Weinstein–Aronszajn formula is discussed in Section 4. The corresponding global Weinstein–Aronszajn formula in terms of modified Fredholm determinants associated with the Birman–Schwinger kernel of  $H$  is the content of Section 5. Both, Sections 4 and 5 are modeled after an exemplary treatment of these topics by Howland [20] in the case where  $H_0$  and  $H$  are self-adjoint. In Section 6 we turn to concrete applications to properly symmetrized (modified) perturbation determinants of non-self-adjoint Dirichlet- and Neumann-type Schrödinger operators in  $L^2(\Omega; d^n x)$  with  $\Omega = (0, \infty)$  in the case  $n = 1$  and rather general open domains  $\Omega \subset \mathbb{R}^n$  with a compact boundary in dimensions  $n = 2, 3$ . The corresponding potentials  $V$  considered are of the form  $V \in L^1((0, \infty); dx)$  for  $n = 1$  and  $V \in L^2(\Omega; d^n x)$  for  $n = 2, 3$ . Our principal result in this section concerns a reduction of the Fredholm determinant of the Birman–Schwinger kernel of  $H$  in  $L^2(\Omega; d^n x)$  to a Fredholm determinant associated with operators in  $L^2(\partial\Omega; d^{n-1}\sigma)$ . The latter should be viewed as a proper multi-dimensional extension of the celebrated result by Jost and Pais [23] concerning the equality of the Jost function (a Wronski determinant) and the associated Fredholm determinant of the underlying Birman–Schwinger kernel. In Section 7 we briefly discuss an application to scattering theory in dimensions  $n = 2, 3$  and re-derive a formula for the Krein spectral shift function (related to the logarithm of the determinant of the scattering matrix) in terms of modified Fredholm determinants of the underlying Birman–Schwinger kernel. We present an alternative derivation of this formula originally due to Cheney [9] for  $n = 2$  and Newton [38] for  $n = 3$  (in the latter case we obtain the result under weaker assumptions on the potential  $V$  than in [38]). Finally, Appendix A summarizes results on Dirichlet and Neumann Laplacians in  $L^2(\Omega; d^n x)$  for a general class of open domains  $\Omega \subseteq \mathbb{R}^n$ ,  $n \geq 2$ , with a compact boundary. We prove the equality of two natural definitions of Dirichlet and Neumann Laplacians for such domains and prove mapping properties between appropriate scales of Sobolev spaces. These results are crucial ingredients in our treatment of modified Fredholm determinants in Section 6, but they also appear to be of independent interest.

We will use the following notation in this paper. Let  $\mathcal{H}$  and  $\mathcal{K}$  be separable complex Hilbert spaces,  $(\cdot, \cdot)_{\mathcal{H}}$  and  $(\cdot, \cdot)_{\mathcal{K}}$  the scalar products in  $\mathcal{H}$  and  $\mathcal{K}$  (linear in the second factor), and  $I_{\mathcal{H}}$  and  $I_{\mathcal{K}}$  the identity operators in  $\mathcal{H}$  and  $\mathcal{K}$ , respectively. Next, let  $T$  be a closed linear operator from  $\text{dom}(T) \subseteq \mathcal{H}$  to  $\text{ran}(T) \subseteq \mathcal{K}$ , with  $\text{dom}(T)$  and  $\text{ran}(T)$  denoting the domain and range of  $T$ . The closure of a closable operator  $S$  is denoted by  $\overline{S}$ . The kernel (null space) of  $T$  is denoted by  $\ker(T)$ . The

spectrum and resolvent set of a closed linear operator in  $\mathcal{H}$  will be denoted by  $\sigma(\cdot)$  and  $\rho(\cdot)$ . The Banach spaces of bounded and compact linear operators in  $\mathcal{H}$  are denoted by  $\mathcal{B}(\mathcal{H})$  and  $\mathcal{B}_\infty(\mathcal{H})$ , respectively. Similarly, the Schatten–von Neumann (trace) ideals will subsequently be denoted by  $\mathcal{B}_p(\mathcal{H})$ ,  $p \in \mathbb{N}$ . Analogous notation  $\mathcal{B}(\mathcal{H}_1, \mathcal{H}_2)$ ,  $\mathcal{B}_\infty(\mathcal{H}_1, \mathcal{H}_2)$ , etc., will be used for bounded, compact, etc., operators between two Hilbert spaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$ . In addition,  $\text{tr}(T)$  denotes the trace of a trace class operator  $T \in \mathcal{B}_1(\mathcal{H})$  and  $\det_p(I_{\mathcal{H}} + S)$  represents the (modified) Fredholm determinant associated with an operator  $S \in \mathcal{B}_p(\mathcal{H})$ ,  $p \in \mathbb{N}$  (for  $p = 1$  we omit the subscript 1). Moreover,  $\mathcal{X}_1 \hookrightarrow \mathcal{X}_2$  denotes the continuous embedding of the Banach space  $\mathcal{X}_1$  into the Banach space  $\mathcal{X}_2$ .

Finally, in Sections 6 and 7 we will introduce various operators of multiplication,  $M_f$ , in  $L^2(\Omega; d^n x)$  by elements  $f \in L^1_{\text{loc}}(\Omega; d^n x)$ , where  $\Omega \subseteq \mathbb{R}^n$  is open and nonempty.

## 2. ABSTRACT PERTURBATION THEORY

In this section, following Kato [24], Konno and Kuroda [28], and Howland [20], we consider a class of factorable non-self-adjoint perturbations of a given unperturbed non-self-adjoint operator. For reasons of completeness we will present proofs of many of the subsequent results even though most of them are only slight deviations from the original proofs in the self-adjoint context.

We start with our first set of hypotheses.

**Hypothesis 2.1.** (i) Suppose that  $H_0: \text{dom}(H_0) \rightarrow \mathcal{H}$ ,  $\text{dom}(H_0) \subseteq \mathcal{H}$  is a densely defined, closed, linear operator in  $\mathcal{H}$  with nonempty resolvent set,

$$\rho(H_0) \neq \emptyset, \quad (2.1)$$

$A: \text{dom}(A) \rightarrow \mathcal{K}$ ,  $\text{dom}(A) \subseteq \mathcal{H}$  a densely defined, closed, linear operator from  $\mathcal{H}$  to  $\mathcal{K}$ , and  $B: \text{dom}(B) \rightarrow \mathcal{K}$ ,  $\text{dom}(B) \subseteq \mathcal{H}$  a densely defined, closed, linear operator from  $\mathcal{H}$  to  $\mathcal{K}$  such that

$$\text{dom}(A) \supseteq \text{dom}(H_0), \quad \text{dom}(B) \supseteq \text{dom}(H_0^*). \quad (2.2)$$

In the following we denote

$$R_0(z) = (H_0 - zI_{\mathcal{H}})^{-1}, \quad z \in \rho(H_0). \quad (2.3)$$

(ii) For some (and hence for all)  $z \in \rho(H_0)$ , the operator  $-AR_0(z)B^*$ , defined on  $\text{dom}(B^*)$ , has a bounded extension in  $\mathcal{K}$ , denoted by  $K(z)$ ,

$$K(z) = -\overline{AR_0(z)B^*} \in \mathcal{B}(\mathcal{K}). \quad (2.4)$$

(iii)  $1 \in \rho(K(z_0))$  for some  $z_0 \in \rho(H_0)$ .

That  $K(z_0) \in \mathcal{B}(\mathcal{K})$  for some  $z_0 \in \rho(H_0)$  implies  $K(z) \in \mathcal{B}(\mathcal{K})$  for all  $z \in \rho(H_0)$  (as mentioned in Hypothesis 2.1 (ii)) is an immediate consequence of (2.2) and the resolvent equation for  $H_0$ .

We emphasize that in the case where  $H_0$  is self-adjoint, the following results in Lemma 2.2, Theorem 2.3, and Remark 2.4 are due to Kato [24] (see also [20], [28]). The more general case we consider here requires only minor modifications. But for the convenience of the reader we will sketch most of the proofs.

**Lemma 2.2.** *Let  $z, z_1, z_2 \in \rho(H_0)$ . Then Hypothesis 2.1 implies the following facts:*

$$AR_0(z) \in \mathcal{B}(\mathcal{H}, \mathcal{K}), \quad \overline{R_0(z)B^*} = [B(H_0^* - \bar{z})^{-1}]^* \in \mathcal{B}(\mathcal{K}, \mathcal{H}), \quad (2.5)$$

$$\overline{R_0(z_1)B^*} - \overline{R_0(z_2)B^*} = (z_1 - z_2)R_0(z_1)\overline{R_0(z_2)B^*} \quad (2.6)$$

$$= (z_1 - z_2)R_0(z_2)\overline{R_0(z_1)B^*}, \quad (2.7)$$

$$K(z) = -A[\overline{R_0(z)B^*}], \quad K(\bar{z})^* = -B[\overline{R_0(\bar{z})^*A^*}], \quad (2.8)$$

$$\text{ran}(\overline{R_0(z)B^*}) \subseteq \text{dom}(A), \quad \text{ran}(\overline{R_0(\bar{z})^*A^*}) \subseteq \text{dom}(B), \quad (2.9)$$

$$K(z_1) - K(z_2) = (z_2 - z_1)AR_0(z_1)\overline{R_0(z_2)B^*} \quad (2.10)$$

$$= (z_2 - z_1)AR_0(z_2)\overline{R_0(z_1)B^*}. \quad (2.11)$$

*Proof.* Equations (2.5) follow from the relations in (2.2) and the Closed Graph Theorem. (2.6) and (2.7) follow from combining (2.5) and the resolvent equation for  $H_0^*$ . Next, let  $f \in \text{dom}(B^*)$ ,  $g \in \text{dom}(A^*)$ , then

$$(\overline{R_0(z)B^*}f, A^*g)_{\mathcal{H}} = (R_0(z)B^*f, A^*g)_{\mathcal{H}} = (AR_0(z)B^*f, g)_{\mathcal{K}} = -(K(z)f, g)_{\mathcal{K}}. \quad (2.12)$$

By continuity this extends to all  $f \in \mathcal{K}$ . Thus,  $-A[\overline{R_0(z)B^*}]f$  exists and equals  $K(z)f$  for all  $f \in \mathcal{K}$ . This proves the first assertions in (2.8) and (2.9). The remaining assertions in (2.8) and (2.9) are of course proved analogously. Multiplying (2.6) and (2.7) by  $A$  from the left and taking into account the first relation in (2.8), then proves (2.10) and (2.11).  $\square$

Next, following Kato [24], one introduces

$$R(z) = R_0(z) - \overline{R_0(z)B^*}[I_{\mathcal{K}} - K(z)]^{-1}AR_0(z), \quad (2.13)$$

$$z \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}.$$

**Theorem 2.3.** *Assume Hypothesis 2.1 and suppose  $z \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}$ . Then,  $R(z)$  defined in (2.13) defines a densely defined, closed, linear operator  $H$  in  $\mathcal{H}$  by*

$$R(z) = (H - zI_{\mathcal{H}})^{-1}. \quad (2.14)$$

Moreover,

$$AR(z), BR(z)^* \in \mathcal{B}(\mathcal{H}, \mathcal{K}) \quad (2.15)$$

and

$$R(z) = R_0(z) - \overline{R(z)B^*}AR_0(z) \quad (2.16)$$

$$= R_0(z) - \overline{R_0(z)B^*}AR(z). \quad (2.17)$$

Finally,  $H$  is an extension of  $(H_0 + B^*A)|_{\text{dom}(H_0) \cap \text{dom}(B^*A)}$  (the latter intersection domain may consist of  $\{0\}$  only),

$$H \supseteq (H_0 + B^*A)|_{\text{dom}(H_0) \cap \text{dom}(B^*A)}. \quad (2.18)$$

*Proof.* Suppose  $z \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}$ . Since by (2.13)

$$AR(z) = [I_{\mathcal{K}} - K(z)]^{-1}AR_0(z), \quad (2.19)$$

$$BR(z)^* = [I_{\mathcal{K}} - K(z)^*]^{-1}BR_0(z)^*, \quad (2.20)$$

$R(z)f = 0$  implies  $AR(z)f = 0$  and hence by (2.19)  $AR_0(z)f = 0$ . The latter implies  $R_0(z)f = 0$  by (2.13) and thus  $f = 0$ . Consequently,

$$\ker(R(z)) = \{0\}. \quad (2.21)$$

Similarly, (2.20) implies

$$\ker(R(z)^*) = \{0\} \text{ and hence } \overline{\text{ran}(R(z))} = \mathcal{H}. \quad (2.22)$$

Next, combining (2.13), the resolvent equation for  $H_0$ , (2.6), (2.7), (2.10), and (2.11) proves the resolvent equation

$$\begin{aligned} R(z_1) - R(z_2) &= (z_1 - z_2)R(z_1)R(z_2), \\ z_1, z_2 &\in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}. \end{aligned} \quad (2.23)$$

Thus,  $R(z)$  is indeed the resolvent of a densely defined, closed, linear operator  $H$  in  $\mathcal{H}$  as claimed in connection with (2.14).

By (2.19) and (2.20),  $AR(z) \in \mathcal{B}(\mathcal{H}, \mathcal{K})$  and  $[BR(\bar{z})^*]^* = \overline{R(z)B^*} \in \mathcal{B}(\mathcal{K}, \mathcal{H})$ , proving (2.15). A combination of (2.13), (2.19), and (2.20) then proves (2.16) and (2.17).

Finally, let  $f \in \text{dom}(H_0) \cap \text{dom}(B^*A)$  and set  $g = (H_0 - zI_{\mathcal{H}})f$ . Then  $R_0(z)g = f$  and by (2.16),  $R(z)g - f = -R(z)B^*Af$ . Thus,  $f \in \text{dom}(H)$  and  $(H - zI_{\mathcal{H}})f = g + B^*Af = (H_0 + B^*A - zI_{\mathcal{H}})f$ , proving (2.18).  $\square$

**Remark 2.4.** (i) Assume that  $H_0$  is self-adjoint in  $\mathcal{H}$ . Then  $H$  is also self-adjoint if

$$(Af, Bg)_{\mathcal{K}} = (Bf, Ag)_{\mathcal{K}} \text{ for all } f, g \in \text{dom}(A) \cap \text{dom}(B). \quad (2.24)$$

(ii) The formalism is symmetric with respect to  $H_0$  and  $H$  in the following sense: The densely defined operator  $-AR(z)B^*$  has a bounded extension to all of  $\mathcal{K}$  for all  $z \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}$ , in particular,

$$I_{\mathcal{K}} - \overline{AR(z)B^*} = [I_{\mathcal{K}} - K(z)]^{-1}, \quad z \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}. \quad (2.25)$$

Moreover,

$$\begin{aligned} R_0(z) &= R(z) + \overline{R(z)B^*}[I_{\mathcal{K}} - \overline{AR(z)B^*}]^{-1}AR(z), \\ z &\in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\} \end{aligned} \quad (2.26)$$

and

$$H_0 \supseteq (H - B^*A)|_{\text{dom}(H) \cap \text{dom}(B^*A)}. \quad (2.27)$$

(iii) The basic hypotheses (2.2) which amount to

$$AR_0(z) \in \mathcal{B}(\mathcal{H}, \mathcal{K}), \quad \overline{R_0(z)B^*} = [B(H_0^* - \bar{z})^{-1}]^* \in \mathcal{B}(\mathcal{K}, \mathcal{H}), \quad z \in \rho(H_0) \quad (2.28)$$

(cf. (2.5)) are more general than a quadratic form perturbation approach which would result in conditions of the form

$$AR_0(z)^{1/2} \in \mathcal{B}(\mathcal{H}, \mathcal{K}), \quad \overline{R_0(z)^{1/2}B^*} = [B(H_0^* - \bar{z})^{-1/2}]^* \in \mathcal{B}(\mathcal{K}, \mathcal{H}), \quad z \in \rho(H_0), \quad (2.29)$$

or even an operator perturbation approach which would involve conditions of the form

$$[B^*A]R_0(z) \in \mathcal{B}(\mathcal{H}), \quad z \in \rho(H_0). \quad (2.30)$$

### 3. A GENERAL BIRMAN–SCHWINGER PRINCIPLE

The principal result in this section represents an abstract version of (a variant of) the Birman–Schwinger principle due to Birman [4] and Schwinger [46] (cf. also [6], [13], [26], [27], [40], [42], [47], and [51]).

We need to strengthen our hypotheses a bit and hence introduce the following assumption:

**Hypothesis 3.1.** In addition to Hypothesis 2.1 we suppose the condition:  
(iv)  $K(z) \in \mathcal{B}_\infty(\mathcal{K})$  for all  $z \in \rho(H_0)$ .

Since by (2.25)

$$-\overline{AR(z)B^*} = [I_{\mathcal{K}} - K(z)]^{-1}K(z) \quad (3.1)$$

$$= -I_{\mathcal{K}} + [I_{\mathcal{K}} - K(z)]^{-1}, \quad (3.2)$$

Hypothesis 3.1 implies that  $-\overline{AR(z)B^*}$  extends to a compact operator in  $\mathcal{K}$  as long as the right-hand side of (3.2) exists.

The following general result is due to Konno and Kuroda [28] in the case where  $H_0$  is self-adjoint. (The more general case presented here requires no modifications but we present a proof for completeness.)

**Theorem 3.2** ([28]). *Assume Hypothesis 3.1 and let  $\lambda_0 \in \rho(H_0)$ . Then,*

$$Hf = \lambda_0 f, \quad 0 \neq f \in \text{dom}(H) \text{ implies } K(\lambda_0)g = g \quad (3.3)$$

where, for fixed  $z_0 \in \{\zeta \in \rho(H_0) \mid 1 \in \rho(K(\zeta))\}$ ,  $z_0 \neq \lambda_0$ ,

$$0 \neq g = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \quad (3.4)$$

$$= (\lambda_0 - z_0)^{-1}Af. \quad (3.5)$$

Conversely,

$$K(\lambda_0)g = g, \quad 0 \neq g \in \mathcal{K} \text{ implies } Hf = \lambda_0 f, \quad (3.6)$$

where

$$0 \neq f = -\overline{R_0(\lambda_0)B^*}g \in \text{dom}(H). \quad (3.7)$$

Moreover,

$$\dim(\ker(H - \lambda_0 I_{\mathcal{H}})) = \dim(\ker(I_{\mathcal{K}} - K(\lambda_0))) < \infty. \quad (3.8)$$

In particular, let  $z \in \rho(H_0)$ , then

$$z \in \rho(H) \text{ if and only if } 1 \in \rho(K(z)). \quad (3.9)$$

*Proof.*  $Hf = \lambda_0 f$ ,  $0 \neq f \in \text{dom}(H)$ , is equivalent to  $f = (\lambda_0 - z_0)R(z_0)f$  and applying (2.13) one obtains after a simple rearrangement that

$$(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f = -(\lambda_0 - z_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f. \quad (3.10)$$

Next, define  $g = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f$ . Then  $g \neq 0$  since otherwise

$$(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f = 0, \quad 0 \neq R_0(z_0)f \in \text{dom}(H_0), \text{ and hence } \lambda_0 \in \sigma(H_0), \quad (3.11)$$

would contradict our hypothesis  $\lambda_0 \in \rho(H_0)$ . Applying  $[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)$  to (3.10) then yields

$$\begin{aligned} [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)(H_0 - \lambda_0 I_{\mathcal{H}})R_0(z_0)f &= [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f = g \\ &= -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\ &= -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}g. \end{aligned} \quad (3.12)$$

Thus, based on (2.10), one infers

$$\begin{aligned} g &= -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(\lambda_0)\overline{R_0(z_0)B^*}g \\ &= [I_{\mathcal{K}} - K(z_0)]^{-1}[K(\lambda_0) - K(z_0)]g \\ &= g - [I_{\mathcal{K}} - K(z_0)]^{-1}[I_{\mathcal{K}} - K(\lambda_0)]g \end{aligned} \quad (3.13)$$

and hence  $K(\lambda_0)g = g$ , proving (3.3). Since  $f = (\lambda_0 - z_0)R(z_0)f$ , using (2.19) one computes

$$\begin{aligned} Af &= (\lambda_0 - z_0)AR(z_0)f \\ &= (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\ &= (\lambda_0 - z_0)g, \end{aligned} \quad (3.14)$$

proving (3.5).

Conversely, suppose  $K(\lambda_0)g = g$ ,  $0 \neq g \in \mathcal{K}$  and define  $f = -\overline{R_0(\lambda_0)B^*}g$ . Then a simple computation using (2.10) shows

$$\begin{aligned} g &= g - [I_{\mathcal{K}} - K(z_0)]^{-1}[I_{\mathcal{K}} - K(\lambda_0)]g \\ &= [I_{\mathcal{K}} - K(z_0)]^{-1}[K(\lambda_0) - K(z_0)]g \\ &= (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f. \end{aligned} \quad (3.15)$$

Thus,  $f \neq 0$  since  $f = 0$  would imply the contradiction  $g = 0$ . Next, inserting the definition of  $f$  into (3.15) yields

$$\begin{aligned} g &= (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\ &= -(\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)\overline{R_0(\lambda_0)B^*}g. \end{aligned} \quad (3.16)$$

Applying  $\overline{R_0(z_0)B^*}$  to (3.16) and taking into account

$$\begin{aligned} \overline{R_0(z_0)B^*}g &= \overline{[R_0(\lambda_0) - (\lambda_0 - z_0)R_0(z_0)R_0(\lambda_0)]B^*}g \\ &= -f + (\lambda_0 - z_0)R_0(z_0)f, \end{aligned} \quad (3.17)$$

a combination of (3.17) and (2.13) yields that

$$\begin{aligned} -f - (z_0 - \lambda_0)R_0(z_0)f &= (\lambda_0 - z_0)\overline{R_0(z_0)B^*}[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f \\ &= (\lambda_0 - z_0)[R_0(z_0) - R(z_0)]f. \end{aligned} \quad (3.18)$$

The latter is equivalent to  $(\lambda_0 - z_0)(H - z_0I_{\mathcal{H}})^{-1}f = f$ . Thus,  $f \in \text{dom}(H)$  and  $Hf = \lambda_0 f$ , proving (3.6).

Since  $K(\lambda_0) \in \mathcal{B}_{\infty}(\mathcal{K})$ , the eigenspace of  $K(\lambda_0)$  corresponding to the eigenvalue 1 is finite-dimensional. The previous considerations established a one-to-one correspondence between the geometric eigenspace of  $K(\lambda_0)$  corresponding to the eigenvalue 1 and the geometric eigenspace of  $H$  corresponding to the eigenvalue  $\lambda_0$ . This proves (3.8).

Finally, (3.8), (2.13), and (2.25) prove (3.9).  $\square$

**Remark 3.3.** It is possible to avoid the compactness assumption in Hypothesis 3.1 in Theorem 3.2 provided that (3.8) is replaced by the statement

$$\text{the subspaces } \ker(H - \lambda_0 I_{\mathcal{H}}) \text{ and } \ker(I_{\mathcal{K}} - K(\lambda_0)) \text{ are isomorphic.} \quad (3.19)$$

(Of course, (3.8) follows from (3.19) provided  $\ker(I_{\mathcal{K}} - K(\lambda_0))$  is finite-dimensional, which in turn follows from Hypothesis 3.1). Indeed, by formula (2.19), we have

$AR(z_0) = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)$ . By formula (3.4), if  $f \neq 0$ , then  $g = AR(z_0)f \neq 0$ , and thus the operator

$$AR(z_0) = [I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0): \ker(H - \lambda_0 I) \rightarrow \ker(K(\lambda_0) - I) \quad (3.20)$$

is injective. By formula (3.16) this operator is also surjective, since each  $g \in \ker(K(\lambda_0) - I)$  belongs to its range,

$$g = (\lambda_0 - z_0)[I_{\mathcal{K}} - K(z_0)]^{-1}AR_0(z_0)f = AR(z_0)f, \quad (3.21)$$

where  $f \in \ker(H - \lambda_0 I)$ .

#### 4. ESSENTIAL SPECTRA AND A LOCAL WEINSTEIN–ARONSZAJN FORMULA

In this section, we closely follow Howland [20] and prove a result which demonstrates the invariance of the essential spectrum. However, since we will extend Howland's result to the non-self-adjoint case, this requires further explanation. Moreover, we will also re-derive Howland's local Weinstein–Aronszajn formula.

**Definition 4.1.** Let  $\Omega \subseteq \mathbb{C}$  be open and connected. Suppose  $\{L(z)\}_{z \in \Omega}$  is a family of compact operators in  $\mathcal{K}$ , which is analytic on  $\Omega$  except for isolated singularities. Following Howland we call  $\{L(z)\}_{z \in \Omega}$  *completely meromorphic* on  $\Omega$  if  $L$  is meromorphic on  $\Omega$  and the principal part of  $L$  at each of its poles is of finite rank.

We start with an auxiliary result due to Steinberg [55] with a modification by Howland [20].

**Lemma 4.2** ([20], [55]). *Let  $\{L(z)\}_{z \in \Omega}$  be an analytic (resp., completely meromorphic) family in  $\mathcal{K}$  on an open connected set  $\Omega \subseteq \mathbb{C}$ . Then for each  $z_0 \in \Omega$  there is a neighborhood  $U(z_0)$  of  $z_0$ , and an analytic  $\mathcal{B}(\mathcal{K})$ -valued function  $M$  on  $U(z_0)$ , such that  $M(z)^{-1} \in \mathcal{B}(\mathcal{K})$  for all  $z \in U(z_0)$  and*

$$M(z)[I_{\mathcal{K}} - L(z)] = I_{\mathcal{K}} - F(z), \quad z \in U(z_0), \quad (4.1)$$

where  $F$  is analytic (resp., meromorphic) on  $U(z_0)$  with  $F(z)$  of finite rank (except at poles) for all  $z \in U(z_0)$ .

The next auxiliary result is due to Ribaric and Vidav [45].

**Lemma 4.3** ([45]). *Let  $\{L(z)\}_{z \in \Omega}$  be a completely meromorphic family in  $\mathcal{K}$  on an open connected set  $\Omega \subseteq \mathbb{C}$ . Then either*

(i)  $I_{\mathcal{K}} - L(z)$  is not boundedly invertible for all  $z \in \Omega$ ,

or

(ii)  $\{[I_{\mathcal{K}} - L(z)]^{-1} - I_{\mathcal{K}}\}_{z \in \Omega}$  is completely meromorphic on  $\Omega$ .

Moreover, we state the following result due to Howland [21].

**Lemma 4.4** ([21]). *Let  $\{L(z)\}_{z \in \Omega}$  be an analytic (resp., meromorphic) family in  $\mathcal{K}$  on an open connected set  $\Omega \subseteq \mathbb{C}$  and suppose that  $L(z)$  has finite rank for each  $z \in \Omega$  (except at poles). Then the following assertions hold:*

(i) *The rank of  $L(z)$  is constant for all  $z \in \Omega$ , except for isolated points where it decreases.*

(ii)  *$\Delta(z) = \det(I_{\mathcal{K}} - L(z))$  and  $\text{tr}(L(z))$  are analytic (resp., meromorphic) for all  $z \in \Omega$ .*

(iii) *Whenever  $\Delta(z) \neq 0$ ,*

$$\Delta'(z)/\Delta(z) = -\text{tr}([I_{\mathcal{K}} - L(z)]^{-1}L'(z)), \quad z \in \Omega. \quad (4.2)$$



We note that it can of course happen that  $\Delta$  vanishes identically on  $\Omega$ .

Next, we introduce the multiplicity function  $m(\cdot, T)$  on  $\mathbb{C}$  associated with a closed, densely defined, linear operator  $T$  in  $\mathcal{H}$  as follows. Suppose  $\lambda_0 \in \mathbb{C}$  is an isolated point in  $\sigma(T)$  and introduce the Riesz projection  $P(\lambda_0, T)$  of  $T$  corresponding to  $\lambda_0$  by

$$P(\lambda_0, T) = -\frac{1}{2\pi i} \oint_{C(\lambda_0; \varepsilon)} d\zeta (T - \zeta I_{\mathcal{H}})^{-1}, \quad (4.3)$$

where  $C(\lambda_0; \varepsilon)$  is a counterclockwise oriented circle centered at  $\lambda_0$  with sufficiently small radius  $\varepsilon > 0$  (excluding the rest of  $\sigma(T)$ ). Then  $m(z, T)$ ,  $z \in \mathbb{C}$ , is defined by

$$m(z, T) = \begin{cases} 0, & \text{if } z \in \rho(T), \\ \dim(\text{ran}(P(z, T))), & \text{if } z \text{ is an isolated eigenvalue of } T \\ & \text{of finite algebraic multiplicity,} \\ +\infty, & \text{otherwise.} \end{cases} \quad (4.4)$$

We note that the dimension of the Riesz projection in (4.3) is finite if and only if  $\lambda_0$  is an isolated eigenvalue of  $T$  of finite algebraic multiplicity (cf. [25, p. 181]). In analogy to the self-adjoint case (but deviating from most definitions in the non-self-adjoint case, see [12, Sect. I.4, Ch. IX]) we now introduce the set

$$\tilde{\sigma}_e(T) = \{\lambda \in \mathbb{C} \mid \lambda \in \sigma(T), \lambda \text{ is not an isolated eigenvalue of } T \\ \text{of finite algebraic multiplicity}\}. \quad (4.5)$$

Of course,  $\tilde{\sigma}_e(T)$  coincides with the essential spectrum of  $T$  if  $T$  is self-adjoint in  $\mathcal{H}$ . In the non-self-adjoint case at hand, the set  $\tilde{\sigma}_e(T)$  is most natural in our study of  $H_0$  and  $H$  as will subsequently be shown. It will also be convenient to introduce the complement of  $\tilde{\sigma}_e(T)$  in  $\mathbb{C}$ ,

$$\begin{aligned} \tilde{\Phi}(T) &= \mathbb{C} \setminus \tilde{\sigma}_e(T) \\ &= \rho(T) \cup \{\lambda \in \mathbb{C} \mid \lambda \text{ is an eigenvalue of } T \text{ of finite algebraic multiplicity}\}. \end{aligned} \quad (4.6)$$

If  $T$  is self-adjoint in  $\mathcal{H}$ ,  $\tilde{\Phi}(T)$  is the Fredholm domain of  $T$ .

If  $\lambda_0 \in \mathbb{C}$  is an isolated eigenvalue of  $T$  of finite algebraic multiplicity, then the singularity structure of the resolvent of  $T$  is of the type

$$\begin{aligned} (T - zI_{\mathcal{H}})^{-1} &= (\lambda_0 - z)^{-1}P(\lambda_0, T) + \sum_{k=1}^{\mu(\lambda_0, T)} (\lambda_0 - z)^{-k-1}(-1)^k D(\lambda_0, T)^k \\ &\quad + \sum_{k=0}^{\infty} (\lambda_0 - z)^k (-1)^k S(\lambda_0, T)^{k+1} \end{aligned} \quad (4.7)$$

for  $z$  in a sufficiently small neighborhood of  $\lambda_0$ . Here

$$D(\lambda_0, T) = (T - \lambda_0 I_{\mathcal{H}})P(\lambda_0, T) = \frac{1}{2\pi i} \oint_{C(\lambda_0; \varepsilon)} d\zeta (\lambda_0 - \zeta)(T - \zeta I_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H}), \quad (4.8)$$

$$S(\lambda_0, T) = -\frac{1}{2\pi i} \oint_{C(\lambda_0; \varepsilon)} d\zeta (\lambda_0 - \zeta)^{-1}(T - \zeta I_{\mathcal{H}})^{-1} \in \mathcal{B}(\mathcal{H}), \quad (4.9)$$

and  $D(\lambda_0, T)$  is nilpotent with its range contained in that of  $P(\lambda_0, T)$ ,

$$D(\lambda_0, T) = P(\lambda_0, T)D(\lambda_0, T) = D(\lambda_0, T)P(\lambda_0, T). \quad (4.10)$$

Moreover,

$$\begin{aligned} S(\lambda_0, T)T &\subset TS(\lambda_0, T), \quad (T - \lambda_0 I_{\mathcal{H}})S(\lambda_0, T) = I_{\mathcal{H}} - P(\lambda_0, T), \\ S(\lambda_0, T)P(\lambda_0, T) &= P(\lambda_0, T)S(\lambda_0, T) = 0. \end{aligned} \quad (4.11)$$

Finally,

$$\mu(\lambda_0, T) \leq m(\lambda_0, T) = \dim(\text{ran}(P(\lambda_0, T))), \quad (4.12)$$

$$\text{tr}(P(\lambda_0, T)) = m(\lambda_0, T), \quad \text{tr}(D(\lambda_0, T)^k) = 0 \text{ for some } k \in \mathbb{N}. \quad (4.13)$$

Next, we need one more notation: Let  $\Omega \subseteq \mathbb{C}$  be open and connected, and let  $f: \Omega \rightarrow \mathbb{C} \cup \{\infty\}$  be meromorphic and not identically vanishing on  $\Omega$ . The multiplicity function  $m(z; f)$ ,  $z \in \Omega$ , is then defined by

$$m(z; f) = \begin{cases} k, & \text{if } z \text{ is a zero of } f \text{ of order } k, \\ -k, & \text{if } z \text{ is a pole of order } k, \\ 0, & \text{otherwise.} \end{cases} \quad (4.14)$$

$$= \frac{1}{2\pi i} \oint_{C(z; \varepsilon)} d\zeta \frac{f'(\zeta)}{f(\zeta)}, \quad z \in \Omega \quad (4.15)$$

for  $\varepsilon > 0$  sufficiently small. If  $f$  vanishes identically on  $\Omega$ , one defines

$$m(z; f) = +\infty, \quad z \in \Omega. \quad (4.16)$$

Here the circle  $C(z; \varepsilon)$  is chosen sufficiently small such that  $C(z; \varepsilon)$  contains no other singularities or zeros of  $f$  except, possibly,  $z$ .

The following result is due to Howland in the case where  $H_0$  and  $H$  are self-adjoint. We will closely follow his strategy of proof and present detailed arguments in the more general situation considered here.

**Theorem 4.5.** *Assume Hypothesis 3.1. Then,*

$$\tilde{\sigma}_e(H) = \tilde{\sigma}_e(H_0). \quad (4.17)$$

*In addition, let  $\lambda_0 \in \mathbb{C} \setminus \tilde{\sigma}_e(H_0)$ . Then there exists a neighborhood  $U(\lambda_0)$  of  $\lambda_0$  and a function  $\Delta(\cdot)$  meromorphic on  $U(\lambda_0)$ , which does not vanish identically, such that the local Weinstein–Aronszajn formula*

$$m(z, H) = m(z, H_0) + m(z; \Delta), \quad z \in U(\lambda_0) \quad (4.18)$$

*holds.*

*Proof.* By (2.10),  $K(\cdot)$  is analytic on  $\rho(H_0)$  and

$$K'(z) = -AR_0(z)[BR_0(z)^*]^*, \quad z \in \rho(H_0). \quad (4.19)$$

Let  $z_0 \in \tilde{\Phi}(H_0)$ , then by (4.7),

$$R_0(z) = (z_0 - z)^{-1}P_0 + \sum_{k=1}^{\mu_0} (z_0 - z)^{-k-1}(-1)^k D_0^k + G_0(z), \quad (4.20)$$

where  $G_0(\cdot)$  is analytic in a neighborhood of  $z_0$ . Since

$$\text{ran}(D_0) \subseteq \text{ran}(P_0) \subset \text{dom}(H_0) \subset \text{dom}(A), \quad (4.21)$$

$AP_0B^*$ ,  $AD_0B^*$ , and  $AG_0(z)B^*$  have compact extensions from  $\text{dom}(B^*)$  to  $\mathcal{K}$ , and the extensions of  $AP_0B^*$  and  $AD_0B^*$  are given by the finite-rank operators  $AP_0[BP_0^*]^*$  and  $\overline{AP_0D_0P_0B^*}$ , respectively. Moreover, it is easy to see that the

extension of  $AG_0(z)B^*$  is analytic near  $z_0$ . Consequently,  $K(\cdot)$  is completely meromorphic on  $\tilde{\Phi}(H_0)$ .

Similarly, by (3.2) and Lemma 4.3,  $-\overline{AR(z)B^*}$  is completely meromorphic on  $\tilde{\Phi}(H_0)$ . Moreover, by (3.2), any singularity  $z_0$  of  $-\overline{AR(z)B^*}$  is an isolated point of  $\sigma(H)$ . Since  $R_0(z)$ ,  $AR_0(z)$ , and  $BR_0(z)$  all have finite-rank principal parts at their poles, (2.13) and (3.2) show that  $R(z)$  also has a finite-rank principal part at  $z_0$ . The latter implies that  $z_0$  is an eigenvalue of  $H$  of finite algebraic multiplicity. Thus,  $\tilde{\Phi}(H_0) \subseteq \tilde{\Phi}(H)$ . Since by Remark 2.4 (ii) this formalism is symmetric with respect to  $H_0$  and  $H$ , one also obtains  $\tilde{\Phi}(H_0) \supseteq \tilde{\Phi}(H)$ , and hence (4.17).

Next, by Lemma 4.2, let  $U_0$  be a neighborhood of  $\lambda_0$  such that

$$M(z)[I_{\mathcal{K}} - K(z)] = I_{\mathcal{K}} - F(z), \quad (4.22)$$

with  $M$  analytic and boundedly invertible on  $U_0$  and some  $F$  meromorphic and of finite rank on  $U_0$ . One defines

$$\Delta(z) = \det(I_{\mathcal{K}} - F(z)), \quad z \in U_0. \quad (4.23)$$

Since by Lemma 4.3,  $[I_{\mathcal{K}} - K(z)]^{-1}$  is meromorphic and  $M(z)$  is boundedly invertible for all  $z \in U_0$ ,  $[I_{\mathcal{K}} - F(z)]^{-1}$  is also meromorphic on  $U_0$ , and hence,  $\Delta(\cdot)$  is not identically zero on  $U_0$ . By Lemma 4.4 (iii) and cyclicity of the trace (i.e.,  $\text{tr}(ST) = \text{tr}(TS)$  for  $S$  and  $T$  bounded operators such that  $ST$  and  $TS$  lie in the trace class, cf. [52, Corollary 3.8]),

$$\begin{aligned} \Delta'(z)/\Delta(z) &= -\text{tr}([I_{\mathcal{K}} - F(z)]^{-1}F'(z)) \\ &= \text{tr}([I_{\mathcal{K}} - K(z)]^{-1}M(z)^{-1}M'(z)[I_{\mathcal{K}} - K(z)] - [I_{\mathcal{K}} - K(z)]^{-1}K'(z)) \\ &= \text{tr}(M(z)^{-1}M'(z) - K'(z)[I_{\mathcal{K}} - K(z)]^{-1}). \end{aligned} \quad (4.24)$$

Let  $z_0 \in U_0$  and  $C(z_0; \varepsilon)$  be a clockwise oriented circle centered at  $z_0$  with sufficiently small radius  $\varepsilon$  (excluding all singularities of  $[I_{\mathcal{K}} - F(z)]^{-1}$ , except, possibly,  $z_0$ ) contained in  $U_0$ . Then,

$$\begin{aligned} m(z_0; \Delta) &= \frac{1}{2\pi i} \oint_{C(z_0; \varepsilon)} d\zeta \frac{\Delta'(\zeta)}{\Delta(\zeta)} \\ &= \frac{1}{2\pi i} \oint_{C(z_0; \varepsilon)} d\zeta \text{tr}(M(\zeta)^{-1}M'(\zeta) - K'(\zeta)[I_{\mathcal{K}} - K(\zeta)]^{-1}). \end{aligned} \quad (4.25)$$

Since  $M$  is analytic and boundedly invertible on  $U_0$ , an interchange of the trace and the integral, using

$$\oint_{C(z_0; \varepsilon)} d\zeta M(\zeta)^{-1}M'(\zeta) = 0 \quad (4.26)$$

and (4.19), then yields

$$\begin{aligned} m(z_0; \Delta) &= \frac{1}{2\pi i} \text{tr} \left( \oint_{C(z_0; \varepsilon)} d\zeta AR_0(\zeta)[BR_0(\zeta)^*]^*[I_{\mathcal{K}} - K(\zeta)]^{-1} \right) \\ &= \frac{1}{2\pi i} \text{tr} \left( \oint_{C(z_0; \varepsilon)} d\zeta AR_0(\zeta)[BR(\zeta)^*]^* \right). \end{aligned} \quad (4.27)$$

Next, for  $\varepsilon > 0$  sufficiently small, one infers from [25, p. 178] (cf. (4.13)) that

$$\begin{aligned} m(z_0, H) - m(z_0, H_0) &= -\frac{1}{2\pi i} \operatorname{tr} \left( \oint_{C(z_0; \varepsilon)} d\zeta [R(\zeta) - R_0(\zeta)] \right) \\ &= \frac{1}{2\pi i} \operatorname{tr} \left( \oint_{C(z_0; \varepsilon)} d\zeta [BR_0(\zeta)^*]^* [I_{\mathcal{K}} - K(\zeta)]^{-1} AR_0(\zeta) \right) \\ &= \frac{1}{2\pi i} \operatorname{tr} \left( \oint_{C(z_0; \varepsilon)} d\zeta [BR(\zeta)^*]^* AR_0(\zeta) \right). \end{aligned} \quad (4.28)$$

At this point we cannot simply change back the order of the trace and the integral and use the cyclicity of the trace to prove equality of (4.27) and (4.28) since now the integrand is not necessarily trace class. But one can prove the equality of (4.27) and (4.28) directly as follows. Writing (cf. (4.7)),

$$AR_0(z) = (z_0 - z)^{-1} \tilde{P}_0 + \sum_{k=1}^{\mu_0} (z_0 - z)^{-k-1} (-1)^k \tilde{D}_0^k + \sum_{k=0}^{\infty} (z_0 - z)^k (-1)^k \tilde{S}_0^{k+1}, \quad (4.29)$$

$$[BR(z)^*]^* = (z_0 - z)^{-1} \tilde{Q}_0 + \sum_{k=1}^{\nu_0} (z_0 - z)^{-k-1} (-1)^k \tilde{E}_0^k + \sum_{k=0}^{\infty} (z_0 - z)^k (-1)^k \tilde{T}_0^{k+1}, \quad (4.30)$$

one obtains

$$\operatorname{res}_{z=z_0} (AR_0(z)[BR(z)^*]^*) = \tilde{P}_0 \tilde{T}_0 + \tilde{S}_0 \tilde{Q}_0 + \sum_{k=1}^{\mu_0} \tilde{D}_0^k \tilde{T}_0^{k+1} + \sum_{k=1}^{\nu_0} \tilde{S}_0^{k+1} \tilde{E}_0^k, \quad (4.31)$$

$$\operatorname{res}_{z=z_0} ([BR(z)^*]^* AR_0(z)) = \tilde{T}_0 \tilde{P}_0 + \tilde{Q}_0 \tilde{S}_0 + \sum_{k=1}^{\mu_0} \tilde{T}_0^{k+1} \tilde{D}_0^k + \sum_{k=1}^{\nu_0} \tilde{E}_0^k \tilde{S}_0^{k+1}. \quad (4.32)$$

Using the cyclicity of the trace and Cauchy's theorem then proves equality of (4.27) and (4.28) and hence (4.18).  $\square$

**Remark 4.6.** Let  $H_0$  be as in Hypothesis 2.1.

(i) Let  $V \in \mathcal{B}_\infty(\mathcal{H})$  and define  $H = H_0 + V$ ,  $\operatorname{dom}(H) = \operatorname{dom}(H_0)$ . Then (4.18) holds identifying  $A = V$ ,  $B = I_{\mathcal{H}}$ , and  $K(z) = VR_0(z)$  in connection with (2.13).

(ii) Let  $V$  be of finite-rank and define  $H = H_0 + V$ ,  $\operatorname{dom}(H) = \operatorname{dom}(H_0)$ . Then (4.18) holds on  $\tilde{\Phi}(H_0)$  with  $\Delta(z) = \det(I_{\mathcal{K}} - K(z))$ ,  $K(z) = VR_0(z)$ ,  $z \in \rho(H_0)$ , and  $U(\lambda_0) = \tilde{\Phi}(H_0)$ .

With the exception of the case discussed in Remark 4.6(ii), Theorem 4.5 has the drawback that it yields a Weinstein–Aronszajn-type formula only locally on  $U(\lambda_0)$ . However, by the same token, the great generality of this formalism, basically assuming only compactness of  $K(\cdot)$ , must be emphasized. In the following section we will present Howland's global Aronszajn–Weinstein formula.

## 5. A GLOBAL WEINSTEIN–ARONSZAJN FORMULA

To this end we introduce a new hypothesis on  $K$ :

**Hypothesis 5.1.** In addition to Hypothesis 3.1 we suppose the condition:

(v) For some  $p \in \mathbb{N}$ ,  $K(z) \in \mathcal{B}_p(\mathcal{K})$  for all  $z \in \rho(H_0)$ .

We denote by  $\|\cdot\|_p$  the norm in  $\mathcal{B}_p(\mathcal{K})$  and by  $\det_p(\cdot)$  the regularized determinant of operators of the type  $I_{\mathcal{K}} - L$ ,  $L \in \mathcal{B}_p(\mathcal{K})$  (cf. [16], [17], [18, Chs. IX–XI], [19, Sect. 4.2], [50], [52, Ch. 9]).

We start by recalling the following result (cf. [19, p. 162–163], [52, p. 107]).

**Lemma 5.2.** *Let  $p \in \mathbb{N}$  and assume that  $\{L(z)\}_{z \in \Omega} \in \mathcal{B}_p(\mathcal{K})$  is a family of  $\mathcal{B}_p(\mathcal{K})$ -analytic operators on  $\Omega$ ,  $\Omega \subseteq \mathbb{C}$  open. Let  $\{P_n\}_{n \in \mathbb{N}}$  be a sequence of orthogonal projections in  $\mathcal{K}$  converging strongly to  $I_{\mathcal{K}}$  as  $n \rightarrow \infty$ . Then, the following limits hold uniformly with respect to  $z$  as  $z$  varies in compact subsets of  $\Omega$ ,*

$$\lim_{n \rightarrow \infty} \|P_n L(z) P_n - L(z)\|_p = 0, \quad (5.1)$$

$$\lim_{n \rightarrow \infty} \det_p(I_{\mathcal{K}} - P_n L(z) P_n) = \det_p(I_{\mathcal{K}} - L(z)), \quad (5.2)$$

$$\lim_{n \rightarrow \infty} \frac{d}{dz} \det_p(I_{\mathcal{K}} - P_n L(z) P_n) = \frac{d}{dz} \det_p(I_{\mathcal{K}} - L(z)). \quad (5.3)$$

So while the situation for analytic  $\mathcal{B}_p(\mathcal{K})$ -valued functions is very satisfactory, there is, however, a problem with meromorphic (even completely meromorphic)  $\mathcal{B}_p(\mathcal{K})$ -valued functions as pointed out by Howland. Indeed, suppose  $L(z)$ ,  $z \in \Omega$ , is meromorphic in  $\Omega$  and of finite rank. Then of course  $\det(I_{\mathcal{K}} - L(\cdot))$  is meromorphic in  $\Omega$ . However, the formula

$$\det_p(I_{\mathcal{K}} - L(z)) = \det(I_{\mathcal{K}} - L(z)) \exp \left[ \operatorname{tr} \left( - \sum_{j=1}^{p-1} j^{-1} L(z)^j \right) \right], \quad z \in \Omega \quad (5.4)$$

shows that  $\det_p(I_{\mathcal{K}} - L(\cdot))$ , for  $p > 1$ , in general, will exhibit essential singularities at poles of  $L$ . To sidestep this difficulty, Howland extends the definition of  $m(\cdot; f)$  in (4.14), (4.15) to functions  $f$  with isolated essential singularities as follows: Suppose  $f$  is meromorphic in  $\Omega$  except at isolated essential singularities. Then we use (4.15) again to define

$$m(z; f) = \frac{1}{2\pi i} \oint_{C(z; \varepsilon)} d\zeta \frac{f'(\zeta)}{f(\zeta)}, \quad z \in \Omega, \quad (5.5)$$

where  $\varepsilon > 0$  is chosen sufficiently small to exclude all singularities and zeros of  $f$  except possibly  $z$ .

Given Lemma 5.2 and the extension of  $m(\cdot; f)$  to meromorphic functions with isolated essential singularities, Howland [20] then proves the following fundamental result (the proof of which is independent of any self-adjointness hypotheses on  $H_0$  and  $H$  and hence omitted here).

**Lemma 5.3** ([20]). *Let  $p \in \mathbb{N}$  and assume that  $\{L(z)\}_{z \in \Omega}$  is a family of  $\mathcal{B}_p(\mathcal{K})$ -valued completely meromorphic operators on  $\Omega$ ,  $\Omega \subseteq \mathbb{C}$  open. Let  $M(z)_{z \in \Omega}$  be a boundedly invertible operator-valued analytic function on  $\Omega$  such that*

$$M(z)[I_{\mathcal{K}} - L(z)] = I_{\mathcal{K}} - F(z), \quad z \in \Omega, \quad (5.6)$$

where  $F(z)$  is meromorphic and of finite rank for all  $z \in \Omega$ . Define

$$\Delta(z) = \det(I_{\mathcal{K}} - F(z)), \quad z \in \Omega, \quad (5.7)$$

and

$$\Delta_p(z) = \det_p(I_{\mathcal{K}} - L(z)), \quad z \in \Omega. \quad (5.8)$$

Then,

$$m(z; \Delta) = m(z; \Delta_p), \quad z \in \Omega. \quad (5.9)$$

Combining Theorem 4.5 and Lemma 5.3 yields Howland's global Weinstein–Aronszajn formula [20] extended to the non-self-adjoint case.

**Theorem 5.4.** *Assume Hypothesis 5.1. Then the global Weinstein–Aronszajn formula*

$$m(z, H) = m(z, H_0) + m(z; \det_p(I_{\mathcal{K}} - K(z))), \quad z \in \tilde{\Phi}(H_0), \quad (5.10)$$

*holds.*

**Remark 5.5.** Let  $H_0$  be as in Hypothesis 2.1, fix  $p \in \mathbb{N}$ , and assume  $VR_0(z) \in \mathcal{B}_p(\mathcal{H})$ . Define  $H = H_0 + V$ ,  $\text{dom}(H) = \text{dom}(H_0)$ . Then (5.10) holds on  $\tilde{\Phi}(H_0)$  with  $K(z) = VR_0(z)$ . In the special case  $p = 1$  this was first obtained by Kuroda [32].

## 6. AN APPLICATION OF PERTURBATION DETERMINANTS TO SCHRÖDINGER OPERATORS IN DIMENSION $n = 1, 2, 3$

In dimension one on a half-line  $(0, \infty)$ , the perturbation determinant associated with the Birman–Schwinger kernel corresponding to a Schrödinger operator with an integrable potential on  $(0, \infty)$  is known to coincide with the corresponding Jost function and hence with a simple Wronski determinant (cf. Lemmas 6.2 and 6.3). This reduction of an infinite-dimensional determinant to a finite-dimensional one is quite remarkable and in this section we intend to give some ideas as to how this fact can be generalized to dimensions two and three.

We start with the one-dimensional situation on the half-line  $\Omega = (0, \infty)$  and introduce the Dirichlet and Neumann Laplacians  $H_{0,+}^D$  and  $H_{0,+}^N$  in  $L^2((0, \infty); dx)$  by

$$\begin{aligned} H_{0,+}^D f &= -f'', \\ f &\in \text{dom}(H_{0,+}^D) = \{g \in L^2((0, \infty); dx) \mid g, g' \in AC([0, R]) \text{ for all } R > 0, \\ &\quad g(0) = 0, g'' \in L^2((0, \infty); dx)\}, \end{aligned} \quad (6.1)$$

$$\begin{aligned} H_{0,+}^N f &= -f'', \\ f &\in \text{dom}(H_{0,+}^N) = \{g \in L^2((0, \infty); dx) \mid g, g' \in AC([0, R]) \text{ for all } R > 0, \\ &\quad g'(0) = 0, g'' \in L^2((0, \infty); dx)\}. \end{aligned} \quad (6.2)$$

Next, we make the following assumption on the potential  $V$ :

**Hypothesis 6.1.** Suppose  $V \in L^1((0, \infty); dx)$ .

Given Hypothesis 6.1, we introduce the perturbed operators  $H_{\Omega}^D$  and  $H_{\Omega}^N$  in  $L^2((0, \infty); dx)$  by

$$\begin{aligned} H_{+}^D f &= -f'' + Vf, \\ f &\in \text{dom}(H_{+}^D) = \{g \in L^2((0, \infty); dx) \mid g, g' \in AC([0, R]) \text{ for all } R > 0, \\ &\quad g(0) = 0, (-g'' + Vg) \in L^2((0, \infty); dx)\}, \end{aligned} \quad (6.3)$$

$$\begin{aligned} H_{+}^N f &= -f'' + Vf, \\ f &\in \text{dom}(H_{+}^N) = \{g \in L^2((0, \infty); dx) \mid g, g' \in AC([0, R]) \text{ for all } R > 0, \\ &\quad g'(0) = 0, (-g'' + Vg) \in L^2((0, \infty); dx)\}. \end{aligned} \quad (6.4)$$

A fundamental system of solutions  $\phi_+^D(z, \cdot)$ ,  $\theta_+^D(z, \cdot)$ , and the Jost solution  $f_+(z, \cdot)$  of

$$-\psi''(z, x) + V\psi(z, x) = z\psi(z, x), \quad z \in \mathbb{C} \setminus \{0\}, \quad x \geq 0, \quad (6.5)$$

are introduced by

$$\phi_+^D(z, x) = z^{-1/2} \sin(z^{1/2}x) + \int_0^x dx' g_+^{(0)}(z, x, x') V(x') \phi_+^D(z, x'), \quad (6.6)$$

$$\theta_+^D(z, x) = \cos(z^{1/2}x) + \int_0^x dx' g_+^{(0)}(z, x, x') V(x') \theta_+^D(z, x'), \quad (6.7)$$

$$f_+(z, x) = e^{iz^{1/2}x} - \int_x^\infty dx' g_+^{(0)}(z, x, x') V(x') f_+(z, x'), \quad (6.8)$$

$$\operatorname{Im}(z^{1/2}) \geq 0, \quad z \in \mathbb{C} \setminus \{0\}, \quad x \geq 0,$$

where

$$g_+^{(0)}(z, x, x') = z^{-1/2} \sin(z^{1/2}(x - x')). \quad (6.9)$$

We introduce

$$u = \exp(i \arg(V)) |V|^{1/2}, \quad v = |V|^{1/2}, \quad \text{so that } V = uv, \quad (6.10)$$

and denote by  $I_+$  the identity operator in  $L^2((0, \infty); dx)$ . In addition, we let

$$W(f, g)(x) = f(x)g'(x) - f'(x)g(x), \quad x \geq 0, \quad (6.11)$$

denote the Wronskian of  $f$  and  $g$ , where  $f, g \in C^1([0, \infty))$ . We also recall our convention to denote by  $M_f$  the operator of multiplication in  $L^2((0, \infty); dx)$  by an element  $f \in L_{\text{loc}}^1((0, \infty); dx)$  (and similarly in the higher-dimensional context in the main part of this section).

The following is a modern formulation of a classical result by Jost and Pais [23].

**Lemma 6.2** ([14, Theorem 4.3]). *Assume Hypothesis 6.1 and  $z \in \mathbb{C} \setminus [0, \infty)$  with  $\operatorname{Im}(z^{1/2}) > 0$ . Then  $\overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v} \in \mathcal{B}_1(L^2((0, \infty); dx))$  and*

$$\begin{aligned} \det(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v}) &= 1 + z^{-1/2} \int_0^\infty dx \sin(z^{1/2}x) V(x) f_+(z, x) \\ &= W(f_+(z, \cdot), \phi_+^D(z, \cdot)) = f_+(z, 0). \end{aligned} \quad (6.12)$$

Performing calculations similar to Section 4 in [14] for the pair of operators  $H_{0,+}^N$  and  $H_+^N$ , one also obtains the following result.

**Lemma 6.3.** *Assume Hypothesis 6.1 and  $z \in \mathbb{C} \setminus [0, \infty)$  with  $\operatorname{Im}(z^{1/2}) > 0$ . Then  $\overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v} \in \mathcal{B}_1(L^2((0, \infty); dx))$  and*

$$\begin{aligned} \det(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v}) &= 1 + iz^{-1/2} \int_0^\infty dx \cos(z^{1/2}x) V(x) f_+(z, x) \\ &= -\frac{W(f_+(z, \cdot), \theta_+^D(z, \cdot))}{iz^{1/2}} = \frac{f'_+(z, 0)}{iz^{1/2}}. \end{aligned} \quad (6.13)$$

We emphasize that (6.12) and (6.13) exhibit the remarkable fact that the Fredholm determinant associated with trace class operators in the infinite-dimensional space  $L^2((0, \infty); dx)$  is reduced to a simple Wronski determinant of  $\mathbb{C}$ -valued distributional solutions of (6.5). This fact goes back to Jost and Pais [23] (see also [14], [37], [39], [41, Sect. 12.1.2], [52, Proposition 5.7], [53], and the extensive literature

cited in these references). The principal aim of this section is to explore possibilities to extend this fact to higher dimensions  $n = 2, 3$ . While a straightforward generalization of (6.12), (6.13) appears to be difficult, we will next derive a formula for the ratio of such determinants which permits a direct extension to dimensions  $n = 2, 3$ .

For this purpose we introduce the boundary trace operators  $\gamma_D$  (Dirichlet trace) and  $\gamma_N$  (Neumann trace) which, in the current one-dimensional half-line situation, are just the functionals,

$$\gamma_D: \begin{cases} C([0, \infty)) \rightarrow \mathbb{C} \\ g \mapsto g(0) \end{cases}, \quad \gamma_N: \begin{cases} C^1([0, \infty)) \rightarrow \mathbb{C} \\ h \mapsto -h'(0) \end{cases}. \quad (6.14)$$

In addition, we denote by  $m_{0,+}^D$ ,  $m_+^D$ ,  $m_{0,+}^N$ , and  $m_+^N$  the Weyl–Titchmarsh  $m$ -functions corresponding to  $H_{0,+}^D$ ,  $H_+^D$ ,  $H_{0,+}^N$ , and  $H_+^N$ , respectively,

$$m_{0,+}^D(z) = iz^{1/2}, \quad m_{0,+}^N(z) = -\frac{1}{m_{0,+}^D(z)} = iz^{-1/2}, \quad (6.15)$$

$$m_+^D(z) = \frac{f'_+(z, 0)}{f_+(z, 0)}, \quad m_+^N(z) = -\frac{1}{m_+^D(z)} = -\frac{f_+(z, 0)}{f'_+(z, 0)}. \quad (6.16)$$

**Theorem 6.4.** *Assume Hypothesis 6.1 and let  $z \in \mathbb{C} \setminus \sigma(H_+^D)$  with  $\text{Im}(z^{1/2}) > 0$ . Then,*

$$\begin{aligned} & \frac{\det(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1}M_v})}{\det(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1}M_v})} \\ &= \frac{W(f_+(z), \phi_+^N(z))}{iz^{1/2}W(f_+(z), \phi_+^D(z))} = \frac{f'_+(z, 0)}{iz^{1/2}f_+(z, 0)} = \frac{m_+^D(z)}{m_{0,+}^D(z)} = \frac{m_{0,+}^N(z)}{m_+^N(z)} \end{aligned} \quad (6.17)$$

$$= 1 - (\gamma_N(H_+^D - zI_+)^{-1}M_V[\gamma_D(H_{0,+}^N - \bar{z}I_+)^{-1}]^*)1. \quad (6.18)$$

*Proof.* We start by noting that  $\sigma(H_{0,+}^D) = \sigma(H_{0,+}^N) = [0, \infty)$ . Applying Lemmas 6.2 and 6.3 and equations (6.15) and (6.16) proves (6.17).

To verify the equality of (6.17) and (6.18) requires some preparations. First we recall that the Green's functions (i.e., integral kernels) of the resolvents of  $H_{0,+}^D$  and  $H_{0,+}^N$  are given by

$$(H_{0,+}^D - zI_+)^{-1}(x, x') = \begin{cases} \frac{\sin(z^{1/2}x)}{z^{1/2}} e^{iz^{1/2}x'}, & 0 \leq x \leq x', \\ \frac{\sin(z^{1/2}x')}{z^{1/2}} e^{iz^{1/2}x}, & 0 \leq x' \leq x, \end{cases} \quad (6.19)$$

$$(H_{0,+}^N - zI_+)^{-1}(x, x') = \begin{cases} \frac{\cos(z^{1/2}x)}{-iz^{1/2}} e^{iz^{1/2}x'}, & 0 \leq x \leq x', \\ \frac{\cos(z^{1/2}x')}{-iz^{1/2}} e^{iz^{1/2}x}, & 0 \leq x' \leq x, \end{cases} \quad (6.20)$$

and hence Krein's formula for the resolvent difference of  $H_{0,+}^D$  and  $H_{0,+}^N$  takes on the simple form

$$\begin{aligned} (H_{0,+}^D - zI_+)^{-1} - (H_{0,+}^N - zI_+)^{-1} &= -iz^{-1/2}(\overline{\psi_{0,+}(z, \cdot)}, \cdot)_{L^2((0, \infty); dx)} \psi_{0,+}(z, \cdot), \\ z &\in \rho(H_{0,+}^D) \cap \rho(H_{0,+}^N), \quad \text{Im}(z^{1/2}) > 0, \end{aligned} \quad (6.21)$$

where we abbreviated

$$\psi_{0,+}(z, x) = e^{iz^{1/2}x}, \quad \text{Im}(z^{1/2}) > 0, \quad x \geq 0. \quad (6.22)$$



We also recall

$$(H_+^D - zI_+)^{-1}(x, x') = \begin{cases} \phi_+^D(z, x)\psi_+(z, x'), & 0 \leq x \leq x', \\ \phi_+^D(z, x')\psi_+(z, x), & 0 \leq x' \leq x, \end{cases} \quad (6.23)$$

where

$$\psi_+(z, x) = \theta_+^D(z, x) + m_+^D(z)\phi_+^D(z, x), \quad z \in \rho(H_+^D), \quad x \geq 0, \quad (6.24)$$

and

$$\psi_+(z, \cdot) = \frac{f_+(z, \cdot)}{f_+(z, 0)} \in L^2((0, \infty); dx), \quad z \in \rho(H_+^D). \quad (6.25)$$

In fact, a standard iteration argument applied to (6.8) shows that

$$|\psi_+(z, x)| \leq C(z)e^{-\operatorname{Im}(z^{1/2})x}, \quad \operatorname{Im}(z^{1/2}) > 0, \quad x \geq 0. \quad (6.26)$$

In addition, we note that

$$\gamma_N(H_{0,+}^D - zI_+)^{-1}g = - \int_0^\infty dx e^{iz^{1/2}x} g(x), \quad g \in L^2((0, \infty); dx), \quad (6.27)$$

$$\gamma_N(H_+^D - zI_+)^{-1}g = - \int_0^\infty dx \psi_+(z, x)g(x), \quad g \in L^2((0, \infty); dx), \quad (6.28)$$

$$\gamma_D(H_{0,+}^N - zI_+)^{-1}f = iz^{-1/2} \int_0^\infty dx e^{iz^{1/2}x} f(x), \quad f \in L^2((0, \infty); dx), \quad (6.29)$$

and hence,

$$([\gamma_D(H_{0,+}^N - \bar{z}I_+)^{-1}]^* c)(\cdot) = icz^{-1/2}\psi_{0,+}(z, \cdot), \quad c \in \mathbb{C}. \quad (6.30)$$

Then Krein's formula (6.21) can be rewritten as

$$(H_{0,+}^D - zI_+)^{-1} - (H_{0,+}^N - zI_+)^{-1} = [\gamma_D(H_{0,+}^N - \bar{z}I_+)^{-1}]^* \gamma_N(H_{0,+}^D - zI_+)^{-1}, \\ z \in \rho(H_{0,+}^D) \cap \rho(H_{0,+}^N), \quad \operatorname{Im}(z^{1/2}) > 0. \quad (6.31)$$

Finally, using the facts (cf. (6.8))

$$f_+(z, 0) = 1 + z^{-1/2} \int_0^\infty dx \sin(z^{1/2}x) V(x) f_+(z, x), \quad (6.32)$$

$$f'_+(z, 0) = iz^{1/2} - \int_0^\infty dx \cos(z^{1/2}x) V(x) f_+(z, x), \quad (6.33)$$

one computes (since  $v \in L^2(\mathbb{R}; dx)$  and  $\psi_+(z, \cdot) \in L^\infty(\mathbb{R}; dx)$ )

$$\begin{aligned} & - [\gamma_N(H_+^D - zI_+)^{-1} M_V [\gamma_D(H_{0,+}^N - \bar{z}I_+)^{-1}]^*] 1 \\ &= -iz^{-1/2} \overline{\gamma_N(H_+^D - zI_+)^{-1} M_u(v\psi_{0,+})(z, \cdot)} \\ &= iz^{-1/2} \int_0^\infty dx e^{iz^{1/2}x} V(x) \psi_+(z, x) \\ &= iz^{-1/2} \int_0^\infty dx \left[ \cos(z^{1/2}x) + iz^{1/2} \frac{\sin(z^{1/2}x)}{z^{1/2}} \right] V(x) \frac{f_+(z, x)}{f_+(z, 0)} \\ &= \frac{i}{z^{1/2} f_+(z, 0)} [iz^{1/2} - f'_+(z, 0) + iz^{1/2}(f_+(z, 0) - 1)] \\ &= \frac{f'_+(z, 0)}{iz^{1/2} f_+(z, 0)} - 1. \end{aligned} \quad (6.34)$$

□

At first sight it may seem unusual to even attempt to prove (6.18) in the one-dimensional case since (6.17) already yields the reduction of a Fredholm determinant to a simple Wronski determinant. However, we will see in Theorem 6.11 that it is precisely (6.18) that permits a straightforward extension to dimensions  $n = 2, 3$ .

**Remark 6.5.** As in Theorem 6.4 we assume Hypothesis 6.1 and suppose  $z \in \mathbb{C} \setminus \sigma(H_+^D)$ . First we note that

$$(H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2} - I_+ \in \mathcal{B}_1(L^2((0, \infty); dx)), \quad (6.35)$$

$$(H_{0,+}^N - zI_+)^{-1/2}(H_+^N - zI_+)(H_{0,+}^N - zI_+)^{-1/2} - I_+ \in \mathcal{B}_1(L^2((0, \infty); dx)). \quad (6.36)$$

Indeed, it follows from the proof of [14, Theorem 4.2] (cf. also Lemma 6.8 below), that

$$\overline{(H_{0,+}^D - zI_+)^{-1/2} M_u}, M_v(H_{0,+}^D - zI_+)^{-1/2} \in \mathcal{B}_2(L^2((0, \infty); dx)), \quad (6.37)$$

and hence,

$$(H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2} - I_+ \quad (6.38)$$

$$= (H_{0,+}^D - zI_+)^{-1/2} M_V(H_{0,+}^D - zI_+)^{-1/2} \in \mathcal{B}_1(L^2((0, \infty); dx)). \quad (6.39)$$

This proves (6.35), and a similar argument yields (6.36). Using the cyclicity of  $\det(\cdot)$ , one can then rewrite the left-hand side of (6.17) as follows,

$$\begin{aligned} & \frac{\det(I_+ + \overline{M_u(H_{0,+}^N - zI_+)^{-1} M_v})}{\det(I_+ + \overline{M_u(H_{0,+}^D - zI_+)^{-1} M_v})} \\ &= \frac{\det(I_+ + (H_{0,+}^N - zI_+)^{-1/2} M_V(H_{0,+}^N - zI_+)^{-1/2})}{\det(I_+ + (H_{0,+}^D - zI_+)^{-1/2} M_V(H_{0,+}^D - zI_+)^{-1/2})} \\ &= \frac{\det((H_{0,+}^N - zI_+)^{-1/2}(H_+^N - zI_+)(H_{0,+}^N - zI_+)^{-1/2})}{\det((H_{0,+}^D - zI_+)^{-1/2}(H_+^D - zI_+)(H_{0,+}^D - zI_+)^{-1/2})}. \end{aligned} \quad (6.40)$$

Equation (6.40) illustrates the kind of symmetrized perturbation determinants underlying Theorem 6.4.

Now we turn to dimensions  $n = 2, 3$ . As a general rule, we will have to replace Fredholm determinants by modified ones.

For the remainder of this section we make the following assumptions on the domain  $\Omega \subset \mathbb{R}^n$ ,  $n = 2, 3$ , and the potential  $V$ :

**Hypothesis 6.6.** Let  $n = 2, 3$ .

(i) Assume that  $\Omega \subset \mathbb{R}^n$  is an open nonempty domain of class  $C^{1,r}$  for some  $(1/2) < r < 1$  with a compact, nonempty boundary,  $\partial\Omega$ . (For details we refer to Appendix A.)

(ii) Suppose that  $V \in L^2(\Omega; d^n x)$ .

First we introduce the boundary trace operator  $\gamma_D^0$  (Dirichlet trace) by

$$\gamma_D^0: C(\overline{\Omega}) \rightarrow C(\partial\Omega), \quad \gamma_D^0 u = u|_{\partial\Omega}. \quad (6.41)$$

Then there exists a bounded, linear operator  $\gamma_D$ ,

$$\gamma_D: H^s(\Omega) \rightarrow H^{s-1/2}(\partial\Omega) \hookrightarrow L^2(\partial\Omega; d^{n-1}\sigma), \quad 1/2 < s < 3/2, \quad (6.42)$$

whose action is compatible with  $\gamma_D^0$ , that is, the two Dirichlet trace operators coincide on the intersection of their domains. It is well-known (see, e.g., [33, Theorem 3.38]), that  $\gamma_D$  is bounded. Here  $d^{n-1}\sigma$  denotes the surface measure on  $\partial\Omega$  and we refer to Appendix A for our notation in connection with Sobolev spaces.

Next, let  $I_{\partial\Omega}$  denote the identity operator in  $L^2(\partial\Omega; d^{n-1}\sigma)$ , and introduce the operator  $\gamma_N$  (Neumann trace) by

$$\gamma_N = \nu \cdot \gamma_D \nabla: H^{s+1}(\Omega) \rightarrow L^2(\partial\Omega; d^{n-1}\sigma), \quad 1/2 < s < 3/2, \quad (6.43)$$

where  $\nu$  denotes outward pointing normal unit vector to  $\partial\Omega$ . It follows from (6.42) that  $\gamma_N$  is also a bounded operator.

Given Hypothesis 6.6(i), we introduce the Dirichlet and Neumann Laplacians  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$  associated with the domain  $\Omega$  as follows,

$$H_{0,\Omega}^D = -\Delta, \quad \text{dom}(H_{0,\Omega}^D) = \{u \in H^2(\Omega) \mid \gamma_D u = 0\}, \quad (6.44)$$

$$H_{0,\Omega}^N = -\Delta, \quad \text{dom}(H_{0,\Omega}^N) = \{u \in H^2(\Omega) \mid \gamma_N u = 0\}. \quad (6.45)$$

In the following we denote by  $I_\Omega$  the identity operator in  $L^2(\Omega; d^n x)$ .

**Lemma 6.7.** *Assume Hypothesis 6.6(i). Then the operators  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$  introduced in (6.44) and (6.45) are nonnegative and self-adjoint in  $\mathcal{H} = L^2(\Omega; d^n x)$  and the following mapping properties hold for all  $q \in \mathbb{R}$  and  $z \in \mathbb{C} \setminus [0, \infty)$ ,*

$$(H_{0,\Omega}^D - zI_\Omega)^{-q}, (H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}(L^2(\Omega; d^n x), H^{2q}(\Omega)). \quad (6.46)$$

The fractional powers in (6.46) (and in subsequent analogous cases such as in (6.54)) are defined via the functional calculus implied by the spectral theorem for self-adjoint operators. For the proof of Lemma 6.7 we refer to Lemmas A.1 and A.2 in Appendix A.

**Lemma 6.8.** *Assume Hypothesis 6.6(i) and let  $(n/2p) < q \leq 1$ ,  $p \geq 2$ ,  $n = 2, 3$ ,  $f \in L^p(\Omega; d^n x)$ , and  $z \in \mathbb{C} \setminus [0, \infty)$ . Then,*

$$M_f(H_{0,\Omega}^D - zI_\Omega)^{-q}, M_f(H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}_p(L^2(\Omega; d^n x)) \quad (6.47)$$

and for some  $c > 0$  (independent of  $z$  and  $f$ )

$$\begin{aligned} & \|M_f(H_{0,\Omega}^D - zI_\Omega)^{-q}\|_{\mathcal{B}_p(L^2(\Omega; d^n x))} + \|M_f(H_{0,\Omega}^N - zI_\Omega)^{-q}\|_{\mathcal{B}_p(L^2(\Omega; d^n x))} \\ & \leq c \|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n; d^n x)} \|f\|_{L^p(\Omega; d^n x)}. \end{aligned} \quad (6.48)$$

*Proof.* We start by noting that under the assumption that  $\Omega$  is a Lipschitz domain, there is a bounded extension operator  $\mathcal{E}$ ,

$$\mathcal{E} \in \mathcal{B}(H^{2q}(\Omega), H^{2q}(\mathbb{R}^n)) \text{ such that } (\mathcal{E}u)|_\Omega = u, \quad u \in H^{2q}(\Omega) \quad (6.49)$$

(see, e.g., [33, Theorem A.4]). Next, denote by  $\mathcal{R}_\Omega$  the restriction operator

$$\mathcal{R}_\Omega: \begin{cases} L^2(\mathbb{R}^n; d^n x) \rightarrow L^2(\Omega; d^n x), \\ u \mapsto u|_\Omega, \end{cases} \quad (6.50)$$

and let  $\tilde{f}$  denote the following extension of  $f$ ,

$$\tilde{f}(x) = \begin{cases} f(x), & x \in \Omega, \\ 0, & x \in \mathbb{R}^n \setminus \Omega, \end{cases} \quad \tilde{f} \in L^p(\mathbb{R}^n; d^n x). \quad (6.51)$$

Then,

$$M_f(H_{0,\Omega}^D - zI_\Omega)^{-q} = \mathcal{R}_\Omega M_{\tilde{f}}(H_0 - zI)^{-q} (H_0 - zI)^q \mathcal{E}(H_{0,\Omega}^D - zI_\Omega)^{-q}, \quad (6.52)$$

where (for simplicity)  $I$  denotes the identity operator in  $L^2(\mathbb{R}^n; d^n x)$  and  $H_0$  denotes the nonnegative self-adjoint operator

$$H_0 = -\Delta, \quad \text{dom}(H_0) = H^2(\mathbb{R}^n) \quad (6.53)$$

in  $L^2(\mathbb{R}^n; d^n x)$ . Utilizing the representation of  $(H_0 - zI)^q$  as the operator of multiplication by  $(|\xi|^2 - z)^q$  in the Fourier space  $L^2(\mathbb{R}^n; d^n \xi)$ , one obtains

$$(H_0 - zI)^q \in \mathcal{B}(H^{2q}(\mathbb{R}^n), L^2(\mathbb{R}^n; d^n x)), \quad (6.54)$$

which together with (6.46) and the mapping property of the extension operator  $\mathcal{E}$  in (6.49) yields

$$(H_0 - zI)^q \mathcal{E}(H_{0,\Omega}^D - zI_\Omega)^{-q} \in \mathcal{B}(L^2(\Omega; d^n x), L^2(\mathbb{R}^n; d^n x)). \quad (6.55)$$

By [52, Theorem 4.1] (or [43, Theorem XI.20]) one also obtains

$$M_{\tilde{f}}(H_0 - zI)^{-q} \in \mathcal{B}_p(L^2(\mathbb{R}^n; d^n x)) \quad (6.56)$$

and

$$\begin{aligned} \|M_{\tilde{f}}(H_0 - zI)^{-q}\|_{\mathcal{B}_p(L^2(\Omega; d^n x))} &\leq c \|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n; d^n x)} \|\tilde{f}\|_{L^p(\mathbb{R}^n; d^n x)} \\ &= c \|(|\cdot|^2 - z)^{-q}\|_{L^p(\mathbb{R}^n; d^n x)} \|f\|_{L^p(\Omega; d^n x)}. \end{aligned} \quad (6.57)$$

Thus, the Dirichlet parts of (6.47) and (6.48) follow from (6.52), (6.55), (6.56), and (6.57).

Similar arguments prove the Neumann parts of (6.47) and (6.48).  $\square$

**Lemma 6.9.** *Assume Hypothesis 6.6(i) and let  $\varepsilon \in (0, 1]$ ,  $n = 2, 3$ , and  $z \in \mathbb{C} \setminus [0, \infty)$ . Then,*

$$\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon}{4}}, \gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon}{4}} \in \mathcal{B}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)). \quad (6.58)$$

*Proof.* It follows from (6.46), that

$$(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon}{4}} \in \mathcal{B}(L^2(\Omega; d^n x), H^{\frac{3+\varepsilon}{2}}(\Omega)), \quad (6.59)$$

$$(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon}{4}} \in \mathcal{B}(L^2(\Omega; d^n x), H^{\frac{1+\varepsilon}{2}}(\Omega)), \quad (6.60)$$

and hence one infers the result from (6.42) and (6.43).  $\square$

**Corollary 6.10.** *Let  $f_1 \in L^{p_1}(\Omega; d^n x)$ ,  $p_1 > 2n$ ,  $f_2 \in L^{p_2}(\Omega; d^n x)$ ,  $p_2 \geq 2$ ,  $p_2 > 2n/3$ ,  $n = 2, 3$ , and  $z \in \mathbb{C} \setminus [0, \infty)$ . Then,*

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{f_1}} \in \mathcal{B}_{p_1}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.61)$$

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1} M_{f_2}} \in \mathcal{B}_{p_2}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)) \quad (6.62)$$

and for some  $c_j(z) > 0$  (independent of  $f_j$ ),  $j = 1, 2$ ,

$$\left\| \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{f_1}} \right\|_{\mathcal{B}_{p_1}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma))} \leq c_1(z) \|f_1\|_{L^{p_1}(\Omega; d^n x)}, \quad (6.63)$$

$$\left\| \overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1} M_{f_2}} \right\|_{\mathcal{B}_{p_2}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma))} \leq c_2(z) \|f_2\|_{L^{p_2}(\Omega; d^n x)}. \quad (6.64)$$

*Proof.* Let  $\varepsilon_1, \varepsilon_2 \in (0, 1)$  be such that  $0 < \varepsilon_1 < 1 - (2n/p_1)$  and  $0 < \varepsilon_2 < \min\{1, 3 - (2n/p_2)\}$ . Then,

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{f_1}} = \gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-\frac{3+\varepsilon_1}{4}} \overline{(H_{0,\Omega}^D - zI_\Omega)^{-\frac{1-\varepsilon_1}{4}}M_{f_1}}, \quad (6.65)$$

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1}M_{f_2}} = \gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-\frac{1+\varepsilon_2}{4}} \overline{(H_{0,\Omega}^N - zI_\Omega)^{-\frac{3-\varepsilon_2}{4}}M_{f_2}}, \quad (6.66)$$

together with Lemmas 6.8 and 6.9 prove the corollary.  $\square$

Next, we introduce the perturbed operators  $H_\Omega^D$  and  $H_\Omega^N$  in  $L^2(\Omega; d^n x)$  as follows. We denote by  $A = M_u$  and  $B = B^* = M_v$  the operators of multiplication by  $u = \exp(i \arg(V)) |V|^{1/2}$  and  $v = |V|^{1/2}$  in  $L^2(\Omega; d^n x)$ , respectively, so that  $M_V = BA = M_u M_v$ . Applying Lemma 6.8 to  $f = u \in L^4(\Omega; d^n x)$  with  $q = 1/2$  yields

$$M_u(H_{0,\Omega}^D - zI_\Omega)^{-1/2}, \overline{(H_{0,\Omega}^D - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_4(L^2(\Omega; d^n x)), \quad z \in \mathbb{C} \setminus [0, \infty), \quad (6.67)$$

$$M_u(H_{0,\Omega}^N - zI_\Omega)^{-1/2}, \overline{(H_{0,\Omega}^N - zI_\Omega)^{-1/2}M_v} \in \mathcal{B}_4(L^2(\Omega; d^n x)), \quad z \in \mathbb{C} \setminus [0, \infty), \quad (6.68)$$

and hence in particular,

$$\text{dom}(A) = \text{dom}(B) \supseteq H^1(\Omega) \supset H^2(\Omega) \supseteq \text{dom}(H_{0,\Omega}^N), \quad (6.69)$$

$$\text{dom}(A) = \text{dom}(B) \supseteq H^1(\Omega) \supseteq H_0^1(\Omega) \supseteq \text{dom}(H_{0,\Omega}^D). \quad (6.70)$$

Thus, Hypothesis 2.1 (i) is satisfied for  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$ . Moreover, (6.67) and (6.68) imply

$$\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \in \mathcal{B}_2(L^2(\Omega; d^n x)), \quad z \in \mathbb{C} \setminus [0, \infty), \quad (6.71)$$

which verifies Hypothesis 2.1 (ii) for  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$ . One verifies Hypothesis 2.1 (iii) by utilizing (6.48) with sufficiently negative  $z < 0$ , such that the  $\mathcal{B}_4$ -norms of the operators in (6.67) and (6.68) are less than 1, and hence, the Hilbert–Schmidt norms of the operators in (6.71) are less than 1. Thus, applying Theorem 2.3 one obtains the densely defined, closed operators  $H_\Omega^D$  and  $H_\Omega^N$  (which are extensions of  $H_{0,\Omega}^D + M_V$  on  $\text{dom}(H_{0,\Omega}^D) \cap \text{dom}(M_V)$  and  $H_{0,\Omega}^N + M_V$  on  $\text{dom}(H_{0,\Omega}^N) \cap \text{dom}(M_V)$ , respectively).

We note in passing that (6.46)–(6.48), (6.58), (6.61)–(6.64), (6.67)–(6.71), etc., extend of course to all  $z$  in the resolvent set of the corresponding operators  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$ .

The following result is a direct extension of the one-dimensional result in Theorem 6.4.

**Theorem 6.11.** *Assume Hypothesis 6.6 and  $z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N))$ . Then,*

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V(H_\Omega^D - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^*} \in \mathcal{B}_1(L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.72)$$

$$\gamma_N(H_\Omega^D - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^* \in \mathcal{B}_2(L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.73)$$

and

$$\begin{aligned}
& \frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v})} \\
&= \det_2(I_{\partial\Omega} - \overline{\gamma_N(H_\Omega^D - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^*}) \\
&\quad \times \exp(\operatorname{tr}(\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V(H_\Omega^D - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^*})).
\end{aligned} \tag{6.74}$$

*Proof.* From the outset we note that the left-hand side of (6.74) is well-defined by (6.71). Let  $z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N))$  and

$$u(x) = \exp(i \arg(V(x))) |V(x)|^{1/2}, \quad v(x) = |V(x)|^{1/2}, \tag{6.75}$$

$$\tilde{u}(x) = \exp(i \arg(V(x))) |V(x)|^{5/6}, \quad \tilde{v}(x) = |V(x)|^{1/6}. \tag{6.76}$$

Next, we introduce

$$K_D(z) = -\overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}, \quad K_N(z) = -\overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v} \tag{6.77}$$

(cf. (2.4)) and utilize the following facts,

$$[I_\Omega - K_D(z)]^{-1} = I_\Omega + K_D(z)[I_\Omega - K_D(z)]^{-1}, \tag{6.78}$$

$$[I_\Omega - K_D(z)]^{-1} \in \mathcal{B}(L^2(\Omega; d^n x)), \tag{6.79}$$

and

$$\begin{aligned}
1 &= \det_2(I_\Omega) = \det_2([I_\Omega - K_D(z)][I_\Omega - K_D(z)]^{-1}) \\
&= \det_2(I_\Omega - K_D(z)) \det_2([I_\Omega - K_D(z)]^{-1}) \exp(\operatorname{tr}(K_D(z)^2[I_\Omega - K_D(z)]^{-1})).
\end{aligned} \tag{6.80}$$

Thus, one obtains

$$\begin{aligned}
& \det_2([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}) \\
&= \det_2(I_\Omega - K_N(z)) \det_2([I_\Omega - K_D(z)]^{-1}) \\
&\quad \times \exp(\operatorname{tr}(K_N(z)K_D(z)[I_\Omega - K_D(z)]^{-1})) \\
&= \frac{\det_2(I_\Omega - K_N(z))}{\det_2(I_\Omega - K_D(z))} \exp(\operatorname{tr}((K_N(z) - K_D(z))K_D(z)[I_\Omega - K_D(z)]^{-1})).
\end{aligned} \tag{6.81}$$

At this point, the left-hand side of (6.74) can be rewritten as

$$\begin{aligned}
& \frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v})} = \frac{\det_2(I_\Omega - K_N(z))}{\det_2(I_\Omega - K_D(z))} \\
&= \det_2([I_\Omega - K_N(z)][I_\Omega - K_D(z)]^{-1}) \\
&\quad \times \exp(\operatorname{tr}((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1})) \\
&= \det_2(I_\Omega + (K_D(z) - K_N(z))[I_\Omega - K_D(z)]^{-1}) \\
&\quad \times \exp(\operatorname{tr}((K_D(z) - K_N(z))K_D(z)[I_\Omega - K_D(z)]^{-1})).
\end{aligned} \tag{6.82}$$

Next, temporarily suppose that  $V(x) \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$ . Using Lemma A.3 (an extension of a result of Nakamura [36, Lemma 6]) and Remark A.5, one finds

$$\begin{aligned} K_D(z) - K_N(z) &= -\overline{M_u \left[ (H_{0,\Omega}^D - zI_\Omega)^{-1} - (H_{0,\Omega}^N - zI_\Omega)^{-1} \right] M_v} \\ &= -\overline{M_u \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} \right]^* \gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}, \quad (6.83) \\ &= -\left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v}. \end{aligned}$$

Thus, inserting (6.83) into (6.82) yields,

$$\begin{aligned} &\frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1} M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v})} \\ &= \det_2 \left( I_\Omega - \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right. \\ &\quad \left. \times \left[ I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right]^{-1} \right) \\ &\quad \times \exp \left( \operatorname{tr} \left( \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right. \right. \\ &\quad \left. \left. \times \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \left[ I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right]^{-1} \right) \right). \quad (6.84) \end{aligned}$$

Then, utilizing Corollary 6.10 with  $p_1 = 12$  and  $p_2 = 12/5$ , one finds,

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \in \mathcal{B}_{12}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.85)$$

$$\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \in \mathcal{B}_{12/5}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.86)$$

and hence using the fact that,

$$\left[ I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right]^{-1} \in \mathcal{B}(L^2(\Omega; d^n x)), \quad z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)), \quad (6.87)$$

one rearranges the terms in (6.84) as follows,

$$\begin{aligned} &\frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1} M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v})} \\ &= \det_2 \left( I_{\partial\Omega} - \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \left[ I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right]^{-1} \right. \\ &\quad \left. \times \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \right) \\ &\quad \times \exp \left( \operatorname{tr} \left( \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right. \right. \\ &\quad \left. \left. \times \left[ I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1} M_v} \right]^{-1} \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \right) \right) \\ &= \det_2 \left( I_{\partial\Omega} - \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\bar{v}}} \left[ I_\Omega + \overline{M_{\bar{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\bar{v}}} \right]^{-1} \right. \\ &\quad \left. \times \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \right) \\ &\quad \times \exp \left( \operatorname{tr} \left( \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\bar{v}}} \overline{M_{\bar{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\bar{v}}} \right. \right. \\ &\quad \left. \left. \times \left[ I_\Omega + \overline{M_{\bar{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1} M_{\bar{v}}} \right]^{-1} \left[ \gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} M_{\bar{u}} \right]^* \right) \right). \quad (6.88) \end{aligned}$$

In the last equality we employed the following simple identities,

$$M_V = M_u M_v = M_{\tilde{u}} M_{\tilde{v}}, \quad (6.89)$$

$$M_v [I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v}]^{-1} M_u = M_{\tilde{v}} [I + \overline{M_{\tilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}}}]^{-1} M_{\tilde{u}}. \quad (6.90)$$

Utilizing (6.88) and the following analog of formula (2.20),

$$\overline{(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}} [I_\Omega + \overline{M_{\tilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}}}]^{-1}} = \overline{(H_\Omega^D - zI_\Omega)^{-1}M_{\tilde{v}}}, \quad (6.91)$$

one arrives at (6.74), subject to the extra assumption  $V \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$ .

Finally, assuming only  $V \in L^2(\Omega; d^n x)$  and utilizing Lemma 6.8 and Corollary 6.10 once again, one obtains

$$M_{\tilde{v}}(H_{0,\Omega}^D - zI_\Omega)^{-1/6} \in \mathcal{B}_{12}(L^2(\Omega; d^n x)), \quad (6.92)$$

$$M_{\tilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-5/6} \in \mathcal{B}_{12/5}(L^2(\Omega; d^n x)), \quad (6.93)$$

$$\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}}} \in \mathcal{B}_{12}(L^2(\Omega; d^n x), L^2(\partial\Omega; d^{n-1}\sigma)), \quad (6.94)$$

$$\overline{\gamma_D(H_{0,\Omega}^N - zI_\Omega)^{-1}M_{\tilde{u}}} \in \mathcal{B}_{12/5}(L^2(L^2(\Omega; d^n x), \partial\Omega; d^{n-1}\sigma)), \quad (6.95)$$

and hence

$$\overline{M_{\tilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}}} \in \mathcal{B}_2(L^2(\Omega; d^n x)). \quad (6.96)$$

Relations (6.92)–(6.96) prove (6.72) and (6.73). Moreover, since

$$[I_\Omega + \overline{M_{\tilde{u}}(H_{0,\Omega}^D - zI_\Omega)^{-1}M_{\tilde{v}}}]^{-1} \in \mathcal{B}(L^2(\Omega; d^n x)), \quad z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D)), \quad (6.97)$$

the left- and the right-hand sides of (6.88), and hence of (6.74), are well-defined for  $V \in L^2(\Omega; d^n x)$ . Thus, using (6.48), (6.63), (6.64), the continuity of  $\det_2(\cdot)$  with respect to the Hilbert–Schmidt norm  $\|\cdot\|_{\mathcal{B}_2(L^2(\Omega; d^n x))}$ , the continuity of  $\text{tr}(\cdot)$  with respect to the trace norm  $\|\cdot\|_{\mathcal{B}_1(L^2(\Omega; d^n x))}$ , and an approximation of  $V \in L^2(\Omega; d^n x)$  by a sequence of potentials  $V_k \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$ ,  $k \in \mathbb{N}$ , in the norm of  $L^2(\Omega; d^n x)$  as  $k \uparrow \infty$ , then extends the result from  $V \in L^2(\Omega; d^n x) \cap L^6(\Omega; d^n x)$  to  $V \in L^2(\Omega; d^n x)$ ,  $n = 2, 3$ .  $\square$

**Remark 6.12.** Thus, a comparison of Theorem 6.11 with the one-dimensional case in Theorem 6.4 shows that the reduction of Fredholm determinants associated with operators in  $L^2((0, \infty); dx)$  to simple Wronski determinants, and hence to Jost functions as first observed by Jost and Pais [23], can be properly extended to higher dimensions and results in a reduction of appropriate ratios of Fredholm determinants associated with operators in  $L^2(\Omega; d^n x)$  to an appropriate Fredholm determinant associated with an operator in  $L^2(\partial\Omega; d^{n-1}\sigma)$ .

**Remark 6.13.** As in Theorem 6.11 we assume Hypothesis 6.6 and suppose  $z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N))$ . First we note that

$$[(H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2} - I_\Omega] \in \mathcal{B}_2(L^2(\Omega; d^n x)), \quad (6.98)$$

$$[(H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2} - I_\Omega] \in \mathcal{B}_2(L^2(\Omega; d^n x)). \quad (6.99)$$



Indeed, by (6.67) and (6.68), one obtains

$$\begin{aligned} & (H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2} - I_\Omega \\ &= (H_{0,\Omega}^D - zI_\Omega)^{-1/2}M_V(H_{0,\Omega}^D - zI_\Omega)^{-1/2} \in \mathcal{B}_2(L^2(\Omega; d^n x)), \end{aligned} \quad (6.100)$$

$$\begin{aligned} & (H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2} - I_\Omega \\ &= (H_{0,\Omega}^N - zI_\Omega)^{-1/2}M_V(H_{0,\Omega}^N - zI_\Omega)^{-1/2} \in \mathcal{B}_2(L^2(\Omega; d^n x)). \end{aligned} \quad (6.101)$$

Thus, using (6.67)–(6.71) and the cyclicity of  $\det_2(\cdot)$ , one rearranges the left-hand side of (6.74) as follows,

$$\begin{aligned} & \frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v})} \\ &= \frac{\det_2(I_\Omega + (H_{0,\Omega}^N - zI_\Omega)^{-1/2}M_V(H_{0,\Omega}^N - zI_\Omega)^{-1/2})}{\det_2(I_\Omega + (H_{0,\Omega}^D - zI_\Omega)^{-1/2}M_V(H_{0,\Omega}^D - zI_\Omega)^{-1/2})} \\ &= \frac{\det_2((H_{0,\Omega}^N - zI_\Omega)^{-1/2}(H_\Omega^N - zI_\Omega)(H_{0,\Omega}^N - zI_\Omega)^{-1/2})}{\det_2((H_{0,\Omega}^D - zI_\Omega)^{-1/2}(H_\Omega^D - zI_\Omega)(H_{0,\Omega}^D - zI_\Omega)^{-1/2})}. \end{aligned} \quad (6.102)$$

Again (6.102) illustrates that symmetrized perturbation determinants underly Theorem 6.11.

**Remark 6.14.** The following observation yields a simple application of formula (6.74). Since by Theorem 3.2, for any  $z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N))$ , one has  $z \in \sigma(H_\Omega^N)$  if and only if  $\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v}) = 0$ , it follows from (6.74) that

$$\begin{aligned} & \text{for all } z \in \mathbb{C} \setminus (\sigma(H_\Omega^D) \cup \sigma(H_{0,\Omega}^D) \cup \sigma(H_{0,\Omega}^N)), \text{ one has } z \in \sigma(H_\Omega^N) \\ & \text{if and only if } \det_2(I_{\partial\Omega} - \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^*}) = 0. \end{aligned} \quad (6.103)$$

One can also prove the following analog of (6.74):

$$\begin{aligned} & \frac{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^D - zI_\Omega)^{-1}M_v})}{\det_2(I_\Omega + \overline{M_u(H_{0,\Omega}^N - zI_\Omega)^{-1}M_v})} \\ &= \det_2(I_{\partial\Omega} + \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V[\gamma_D(H_\Omega^N - \bar{z}I_\Omega)^{-1}]^*}) \\ & \quad \times \exp(-\operatorname{tr}(\overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V(H_\Omega^N - zI_\Omega)^{-1}M_V[\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^*})). \end{aligned} \quad (6.104)$$

Then, proceeding as before, one obtains

$$\begin{aligned} & \text{for all } z \in \mathbb{C} \setminus (\sigma(H_\Omega^N) \cup \sigma(H_{0,\Omega}^N) \cup \sigma(H_{0,\Omega}^D)), \text{ one has } z \in \sigma(H_\Omega^D) \\ & \text{if and only if } \det_2(I_{\partial\Omega} + \overline{\gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}M_V[\gamma_D(H_\Omega^N - \bar{z}I_\Omega)^{-1}]^*}) = 0. \end{aligned} \quad (6.105)$$

## 7. AN APPLICATION TO SCATTERING THEORY

In this section we relate Krein's spectral shift function and hence the determinant of the scattering operator in connection with quantum mechanical scattering theory in dimensions  $n = 2, 3$  with appropriate modified Fredholm determinants.

The results of this section are not new, they were first derived for  $n = 3$  by Newton [38] and subsequently for  $n = 2$  by Cheney [9]. However, since our method of

proof nicely illustrates the use of infinite determinants in connection with scattering theory and is different from that in [38] and [9], and moreover, since our derivation in the case  $n = 3$  is performed under slightly more general hypotheses than in [38], we thought it worthwhile to include it at this point.

**Hypothesis 7.1.** Fix  $\delta > 0$ . Suppose  $V \in \mathcal{R}_{2,\delta}$  for  $n = 2$  and  $V \in L^1(\mathbb{R}^3; d^3x) \cap \mathcal{R}_3$  for  $n = 3$ , where

$$\mathcal{R}_{2,\delta} = \{V: \mathbb{R}^2 \rightarrow \mathbb{R} \text{ measurable} \mid V^{1+\delta}, (1 + |\cdot|^\delta)V \in L^1(\mathbb{R}^2; d^2x)\}, \quad (7.1)$$

$$\mathcal{R}_3 = \left\{ V: \mathbb{R}^3 \rightarrow \mathbb{R} \text{ measurable} \mid \int_{\mathbb{R}^6} d^3x d^3x' |V(x)| |V(x')| |x - x'|^{-2} < \infty \right\}. \quad (7.2)$$

We introduce  $H_0$  as the following nonnegative self-adjoint operator in the Hilbert space  $L^2(\mathbb{R}^n; d^n x)$ ,

$$H_0 = -\Delta, \quad \text{dom}(H_0) = H^2(\mathbb{R}^n), \quad n = 2, 3. \quad (7.3)$$

Moreover, let  $A = M_u$  and  $B = B^* = M_v$  denote the operators of multiplication by  $u = \text{sign}(V)|V|^{1/2}$  and  $v = |V|^{1/2}$  in  $L^2(\mathbb{R}^n; d^n x)$ , respectively, so that  $M_V = BA = M_u M_v$ . Then, (cf. [48, Theorem I.21] for  $n = 3$  and [49] for  $n = 2$ ),

$$\text{dom}(A) = \text{dom}(B) \supseteq H^1(\mathbb{R}^n) \supset \text{dom}(H_0), \quad (7.4)$$

and hence, Hypothesis 2.1 (i) is satisfied for  $H_0$ . It follows from Hypothesis 7.1 that

$$\overline{M_u(H_0 - zI)^{-1}M_v} \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \quad z \in \mathbb{C} \setminus [0, \infty), \quad (7.5)$$

where  $I$  now denotes the identity operator in  $L^2(\mathbb{R}^n; d^n x)$ , and hence, Hypothesis 2.1 (ii) is satisfied. Taking  $z \in \mathbb{C} \setminus [0, \infty)$  with a sufficiently large absolute value, one also verifies Hypothesis 2.1 (iii). Thus, applying Theorem 2.3 and Remark 2.4 (i), one obtains a self-adjoint operator  $H$  (which is an extension of  $H_0 + V$  on  $\text{dom}(H_0) \cap \text{dom}(V)$ ).

**Theorem 7.2.** Assume Hypothesis 7.1 and let  $z \in \mathbb{C} \setminus \sigma(H)$  and  $n = 2, 3$ . Then,

$$(H - zI)^{-1} - (H_0 - zI)^{-1} \in \mathcal{B}_1(L^2(\mathbb{R}^n; d^n x)), \quad (7.6)$$

and there is a unique real-valued spectral shift function

$$\xi(\cdot, H, H_0) \in L^1(\mathbb{R}; (1 + \lambda^2)^{-1} d\lambda) \quad (7.7)$$

such that  $\xi(\lambda, H, H_0) = 0$  for  $\lambda < \inf(\sigma(H))$ , and

$$\text{tr}((H - zI)^{-1} - (H_0 - zI)^{-1}) = - \int_{\sigma(H)} \frac{d\lambda \xi(\lambda, H, H_0)}{(\lambda - z)^2}. \quad (7.8)$$

We recall that  $\xi(\cdot, H, H_0)$  is called the spectral shift function for the pair of self-adjoint operators  $(H, H_0)$ . For background information on  $\xi(\cdot, H, H_0)$  and its connection with the scattering operator at fixed energy, we refer, for instance, to [3, Sect. 19.1], [5], [7], [62, Ch. 8].

**Lemma 7.3.** Assume Hypothesis 7.1 and let  $z \in \mathbb{C} \setminus \sigma(H)$  and  $n = 2, 3$ . Then,

$$\overline{M_u(H_0 - zI)^{-1}M_v} \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \quad (7.9)$$

$$(H_0 - zI)^{-1}M_V(H_0 - zI)^{-1} \in \mathcal{B}_1(L^2(\mathbb{R}^n; d^n x)), \quad (7.10)$$

and

$$\begin{aligned} & \frac{d}{dz} \ln(\det_2(I + \overline{M_u(H_0 - zI)^{-1}M_v})) \\ &= -\operatorname{tr}((H - zI)^{-1} - (H_0 - zI)^{-1} + (H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}). \end{aligned} \quad (7.11)$$

The key ingredient in proving (7.6) is the fact that

$$M_u(H_0 - zI)^{-1}, \overline{(H_0 - zI)^{-1}M_v} \in \mathcal{B}_2(L^2(\mathbb{R}^n; d^n x)), \quad z \in \mathbb{C} \setminus [0, \infty), \quad n = 2, 3. \quad (7.12)$$

This follows from either [52, Theorem 4.1] (or [43, Theorem XI.20]), or explicitly by an inspection of the corresponding integral kernels. For instance, the one for  $M_u(H_0 - zI)^{-1}$  reads:

$$\begin{aligned} (M_u(H_0 - zI)^{-1})(x, x') &= \begin{cases} u(x)(i/4)H_0^{(1)}(z^{1/2}|x - x'|), & x \neq x', \quad x, x' \in \mathbb{R}^2, \\ u(x)e^{iz^{1/2}|x - x'|}/[4\pi|x - x'|], & x \neq x', \quad x, x' \in \mathbb{R}^3, \end{cases} \\ & \quad z \in \mathbb{C} \setminus [0, \infty), \quad \operatorname{Im}(z^{1/2}) > 0, \end{aligned} \quad (7.13)$$

where  $H_0^{(1)}(\cdot)$  denotes the Hankel function of order zero and first kind (see, e.g., [1, Sect. 9.1]). Hence, one only needs to apply equation (2.13) to conclude (7.6) and hence (7.10) (by factoring  $M_V = M_u M_v$ ). (We note that (7.6) is proved in [43, Sect. XI.6] and [48, Theorem II.37] for  $n = 3$ .) Relation (7.9) is then clear from  $V \in \mathcal{R}_3$  for  $n = 3$  and follows from [49] for  $n = 2$ . Equation (7.11) is discussed in [8] for  $n = 2, 3$ . The trace formula (7.8) is a celebrated result of Krein [29], [30]; detailed accounts of it can be found in [3, Sect. 19.1.5], [7], [31], [62, Ch. 8].

**Lemma 7.4.** *Assume Hypothesis 7.1. Then the following formula holds for a.e.  $\lambda \in \mathbb{R}$ ,*

$$\begin{aligned} 2\pi i \xi(\lambda, H, H_0) &= \ln \left( \frac{\det_2(I + \overline{M_u(H_0 - (\lambda + i0)I)^{-1}M_v})}{\det_2(I + \overline{M_u(H_0 - (\lambda - i0)I)^{-1}M_v})} \right) \\ &+ \frac{i}{2\pi} \int_{\mathbb{R}^n} d^n x V(x) \times \begin{cases} \pi, & \lambda > 0, \quad n = 2, \\ \lambda^{1/2}, & \lambda > 0, \quad n = 3, \\ 0, & \lambda \leq 0, \quad n = 2, 3. \end{cases} \end{aligned} \quad (7.14)$$

*Proof.* It follows from Theorem 7.2 and Lemma 7.3, that for  $z \in \mathbb{C} \setminus \sigma(H)$ ,

$$\begin{aligned} \int_{\mathbb{R}} \frac{d\lambda \xi(\lambda, H, H_0)}{(\lambda - z)^2} &= \frac{d}{dz} \ln(\det_2(I + \overline{M_u(H_0 - zI)^{-1}M_v})) \\ &+ \operatorname{tr}((H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}). \end{aligned} \quad (7.15)$$

First, we rewrite the left-hand side of (7.15). Since  $\xi(\cdot, H, H_0) \in L^1(\mathbb{R}; \frac{d\lambda}{1+\lambda^2})$ , one has the following formula,

$$\int_{\mathbb{R}} \frac{d\lambda \xi(\lambda, H, H_0)}{(\lambda - z)^2} = \frac{d}{dz} \int_{\mathbb{R}} d\lambda \xi(\lambda, H, H_0) \left( \frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right), \quad z \in \mathbb{C} \setminus \sigma(H). \quad (7.16)$$

Next, we compute the second term on the right-hand side of (7.15). By (7.12) and the cyclicity of the trace,

$$\operatorname{tr}((H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}) = \operatorname{tr}(\overline{M_u(H_0 - zI)^{-2}M_v}), \quad z \in \mathbb{C} \setminus [0, \infty). \quad (7.17)$$

Then  $\overline{M_u(H_0 - zI)^{-2}M_v} = \overline{M_u \frac{d}{dz}(H_0 - zI)^{-1}M_v}$  has the integral kernel

$$\begin{aligned} (\overline{M_u(H_0 - zI)^{-2}M_v})(x, x') = & \begin{cases} u(x) \frac{iH_0^{(1)'}(z^{1/2}|x-x'|)|x-x'|}{8z^{1/2}} v(x'), & x, x' \in \mathbb{R}^2, \\ u(x) \frac{i \exp(iz^{1/2}|x-x'|)}{8\pi z^{1/2}} v(x'), & x, x' \in \mathbb{R}^3, \\ x \neq x', z \in \mathbb{C} \setminus [0, \infty), \operatorname{Im}(z^{1/2}) > 0, \end{cases} \end{aligned} \quad (7.18)$$

and hence, utilizing [11, p. 1086], one computes for  $z \in \mathbb{C} \setminus [0, \infty)$ ,

$$\begin{aligned} \operatorname{tr}((H_0 - zI)^{-1}M_V(H_0 - zI)^{-1}) &= \frac{1}{4\pi} \int_{\mathbb{R}^n} d^n x V(x) \times \begin{cases} -z^{-1}, & n = 2 \\ i(2z^{1/2})^{-1}, & n = 3 \end{cases} \\ &= \frac{1}{4\pi} \int_{\mathbb{R}^n} d^n x V(x) \times \frac{d}{dz} \begin{cases} -\ln(z), & n = 2, \\ iz^{1/2}, & n = 3. \end{cases} \end{aligned} \quad (7.19)$$

Finally, using (7.15), (7.16), and (7.19), one obtains for  $z \in \mathbb{C} \setminus \sigma(H)$ ,

$$\begin{aligned} & \int_{\mathbb{R}} d\lambda \xi(\lambda, H, H_0) \left( \frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right) + C \\ &= \ln(\det_2(I + \overline{M_u(H_0 - zI)^{-1}M_v})) + \frac{1}{4\pi} \int_{\mathbb{R}^n} d^n x V(x) \times \begin{cases} -\ln(z), & n = 2, \\ iz^{1/2}, & n = 3, \end{cases} \end{aligned} \quad (7.20)$$

where  $C \in \mathbb{C}$  denotes an appropriate constant. To complete the proof we digress for a moment and recall the Stieltjes inversion formula for Herglotz functions  $m$  (i.e., analytic maps  $m: \mathbb{C}_+ \rightarrow \mathbb{C}_+$ , where  $\mathbb{C}_+$  denotes the open complex upper half-plane). Such functions  $m$  permit the Nevanlinna, respectively, Riesz-Herglotz representation

$$\begin{aligned} m(z) &= c + dz + \int_{\mathbb{R}} d\omega(\lambda) \left( \frac{1}{\lambda - z} - \frac{\lambda}{1 + \lambda^2} \right), \quad z \in \mathbb{C}_+, \\ c &= \operatorname{Re}[m(i)], \quad d = \lim_{\eta \uparrow \infty} m(i\eta)/(i\eta) \geq 0, \end{aligned} \quad (7.21)$$

with a nonnegative measure  $d\omega$  on  $\mathbb{R}$  satisfying

$$\int_{\mathbb{R}} \frac{d\omega(\lambda)}{1 + \lambda^2} < \infty. \quad (7.22)$$

The absolutely continuous part  $d\omega_{ac}$  of  $d\omega$  with respect to Lebesgue measure  $d\lambda$  on  $\mathbb{R}$  is then known to be given by

$$d\omega_{ac}(\lambda) = \pi^{-1} \operatorname{Im}[m(\lambda + i0)] d\lambda. \quad (7.23)$$

In addition, one extends  $m$  to the open lower complex half-plane  $\mathbb{C}_-$  by

$$m(z) = \overline{m(\bar{z})}, \quad z \in \mathbb{C}_-. \quad (7.24)$$

(We refer, e.g., to [2, Sect. 69] for details on (7.21)–(7.24).) Thus, in order to apply (7.21)–(7.24) to the computation of  $\xi(\cdot, H, H_0)$  in (7.20) it suffices to decompose  $\xi(\cdot, H, H_0) = \xi_+(\cdot, H, H_0) - \xi_-(\cdot, H, H_0)$  into its positive and negative parts  $\xi_{\pm}(\cdot, H, H_0) \geq 0$  and separately consider the absolutely continuous measures  $\xi_{\pm}(\cdot, H, H_0)d\lambda$ . Thus, letting  $z = \lambda \pm i\varepsilon$ , taking the limit  $\varepsilon \downarrow 0$  in (7.20), and subtracting the corresponding results, yields (7.14).  $\square$

We conclude with the following result:

**Corollary 7.5.** *Assume Hypothesis 7.1. Then, for a.e.  $\lambda > 0$ ,*

$$\begin{aligned} \det(S(\lambda)) &= \frac{\det_2(I + \overline{M_u}(H_0 - (\lambda - i0)I)^{-1}M_v)}{\det_2(I + \overline{M_u}(H_0 - (\lambda + i0)I)^{-1}M_v)} \\ &\quad \times \begin{cases} \exp\left(-\frac{i}{2} \int_{\mathbb{R}^n} d^n x V(x)\right), & n = 2, \\ \exp\left(-\frac{i\lambda^{1/2}}{2\pi} \int_{\mathbb{R}^n} d^n x V(x)\right), & n = 3. \end{cases} \end{aligned} \quad (7.25)$$

*Proof.* Hypothesis 7.1 implies that the scattering operator  $S(\lambda)$  at fixed energy  $\lambda > 0$  in  $L^2(S^{n-1}; d^{n-1}\omega)$  satisfies

$$[S(\lambda) - I] \in \mathcal{B}_1(L^2(S^{n-1}; d^{n-1}\omega)) \text{ for a.e. } \lambda > 0 \quad (7.26)$$

and

$$\det(S(\lambda)) = \exp(-2\pi i \xi(\lambda, H, H_0)) \text{ for a.e. } \lambda > 0 \quad (7.27)$$

(cf., e.g., [3, Sects. 19.1.4, 19.1.5], [5], [7], [62, Ch. 8]), where  $S^{n-1}$  denotes the unit sphere in  $\mathbb{R}^n$  and  $d^{n-1}\omega$  the corresponding surface measure on  $S^{n-1}$ . Relation (7.25) then follows from Lemma 7.4 and (7.27).  $\square$

We note again that Corollary 7.5 was derived earlier using different means by Cheney [9] for  $n = 2$  and by Newton [38] for  $n = 3$ . (The stronger conditions  $V \in L^2(\mathbb{R}^3; dx^3)$  and the existence of  $a > 0$  and  $0 < C < \infty$  such that for all  $y \in \mathbb{R}^3$ ,  $\int_{\mathbb{R}^3} d^3x |V(x)|[(|x| + |y| + a)/(|x - y|)]^2 \leq C$ , are assumed in [38].)

#### APPENDIX A. PROPERTIES OF THE DIRICHLET AND NEUMANN LAPLACIANS

The purpose of this appendix is to derive some basic domain properties of Dirichlet and Neumann Laplacians on  $C^{1,r}$ -domains  $\Omega \subset \mathbb{R}^n$  and to prove Lemma 6.7. Throughout this appendix we assume  $n \geq 2$ , but we note that  $n$  is restricted to  $n = 2, 3$  in Sections 6 and 7.

In this manuscript we use the following notation for the standard Sobolev Hilbert spaces ( $s \in \mathbb{R}$ ),

$$H^s(\mathbb{R}^n) = \left\{ U \in \mathcal{S}(\mathbb{R}^n)^* \mid \|U\|_{H^s(\mathbb{R}^n)}^2 = \int_{\mathbb{R}^n} d^n \xi |\widehat{U}(\xi)|^2 (1 + |\xi|^2)^s < \infty \right\}, \quad (\text{A.1})$$

$$H^s(\Omega) = \{u \in C_0^\infty(\Omega)^* \mid u = U|_\Omega \text{ for some } U \in H^s(\mathbb{R}^n)\}, \quad (\text{A.2})$$

$$H_0^s(\Omega) = \text{the closure of } C_0^\infty(\Omega) \text{ in the norm of } H^s(\Omega). \quad (\text{A.3})$$

Here  $C_0^\infty(\Omega)^*$  denotes the usual set of distributions on  $\Omega \subseteq \mathbb{R}^n$ ,  $\Omega$  open and nonempty,  $\mathcal{S}(\mathbb{R}^n)^*$  is the space of tempered distributions on  $\mathbb{R}^n$ , and  $\widehat{U}$  denotes the Fourier transform of  $U \in \mathcal{S}(\mathbb{R}^n)^*$ . It is then immediate that

$$H^{s_0}(\Omega) \hookrightarrow H^{s_1}(\Omega) \text{ whenever } -\infty < s_0 \leq s_1 < +\infty, \quad (\text{A.4})$$

continuously and densely.

Before we present a proof of Lemma 6.7, we recall the definition of a  $C^{1,r}$ -domain  $\Omega \subseteq \mathbb{R}^n$ ,  $\Omega$  open and nonempty, for convenience of the reader: Let  $\mathcal{N}$  be a space of real-valued functions in  $\mathbb{R}^{n-1}$ . One calls a bounded domain  $\Omega \subset \mathbb{R}^n$  of class  $\mathcal{N}$  if there exists a finite open covering  $\{\mathcal{O}_j\}_{1 \leq j \leq N}$  of the boundary  $\partial\Omega$  of  $\Omega$  with the property that, for every  $j \in \{1, \dots, N\}$ ,  $\mathcal{O}_j \cap \Omega$  coincides with the portion of  $\mathcal{O}_j$  lying in the over-graph of a function  $\varphi_j \in \mathcal{N}$  (considered in a new system of coordinates

obtained from the original one via a rigid motion). Two special cases are going to play a particularly important role in the sequel. First, if  $\mathcal{N}$  is  $\text{Lip}(\mathbb{R}^{n-1})$ , the space of real-valued functions satisfying a (global) Lipschitz condition in  $\mathbb{R}^{n-1}$ , we shall refer to  $\Omega$  as being a Lipschitz domain; cf. [54, p. 189], where such domains are called “minimally smooth”. Second, corresponding to the case when  $\mathcal{N}$  is the subspace of  $\text{Lip}(\mathbb{R}^{n-1})$  consisting of functions whose first-order derivatives satisfy a (global) Hölder condition of order  $r \in (0, 1)$ , we shall say that  $\Omega$  is of class  $C^{1,r}$ . The classical theorem of Rademacher of almost everywhere differentiability of Lipschitz functions ensures that, for any Lipschitz domain  $\Omega$ , the surface measure  $d\sigma$  is well-defined on  $\partial\Omega$  and that there exists an outward pointing normal vector  $\nu$  at almost every point of  $\partial\Omega$ . For a Lipschitz domain  $\Omega \subset \mathbb{R}^n$  it is known that

$$(H^s(\Omega))^* = H^{-s}(\Omega), \quad -\frac{1}{2} < s < \frac{1}{2}. \quad (\text{A.5})$$

See [59] for this and other related properties.

Next, assume that  $\Omega \subset \mathbb{R}^n$  is the domain lying above the graph of a function  $\varphi : \mathbb{R}^{n-1} \rightarrow \mathbb{R}$  of class  $C^{1,r}$ . Then for  $0 \leq s < 1 + r$ , the Sobolev space  $H^s(\partial\Omega)$  consists of functions  $f \in L^2(\partial\Omega; d^{n-1}\sigma)$  such that  $f(x', \varphi(x'))$ , as function of  $x' \in \mathbb{R}^{n-1}$ , belongs to  $H^s(\mathbb{R}^{n-1})$ . This definition is easily adapted to the case when  $\Omega$  is domain of class  $C^{1,r}$  whose boundary is compact, by using a smooth partition of unity. Finally, for  $-1 - r < s < 0$ , we set  $H^s(\partial\Omega) = (H^{-s}(\partial\Omega))^*$ . For additional background information in this context we refer, for instance, to [33, Ch. 3], [61, Sect. I.4.2].

Assuming Hypothesis 6.6 (i) (i.e.,  $\Omega$  is an open nonempty  $C^{1,r}$ -domain for some  $(1/2) < r < 1$  with compact boundary  $\partial\Omega$ ), we introduce the Dirichlet and Neumann Laplacians  $\tilde{H}_{0,\Omega}^D$  and  $\tilde{H}_{0,\Omega}^N$  associated with the domain  $\Omega$  as the unique self-adjoint operators on  $L^2(\Omega; d^n x)$  whose quadratic form equals  $q(f, g) = \int_{\Omega} d^n x \nabla f \cdot \nabla g$  with the form domains  $H_0^1(\Omega)$  and  $H^1(\Omega)$ , respectively. Then,

$$\begin{aligned} \text{dom}(\tilde{H}_{0,\Omega}^D) &= \{u \in H_0^1(\Omega) \mid \text{there exists } f \in L^2(\Omega; d^n x) \text{ such that} \\ &\quad q(u, v) = (f, v)_{L^2(\Omega; d^n x)} \text{ for all } v \in H_0^1(\Omega)\}, \end{aligned} \quad (\text{A.6})$$

$$\begin{aligned} \text{dom}(\tilde{H}_{0,\Omega}^N) &= \{u \in H^1(\Omega) \mid \text{there exists } f \in L^2(\Omega; d^n x) \text{ such that} \\ &\quad q(u, v) = (f, v)_{L^2(\Omega; d^n x)} \text{ for all } v \in H^1(\Omega)\}, \end{aligned} \quad (\text{A.7})$$

with  $(\cdot, \cdot)_{L^2(\Omega; d^n x)}$  denoting the scalar product in  $L^2(\Omega; d^n x)$ . Equivalently, we introduce the densely defined closed linear operators

$$D = \nabla, \text{ dom}(D) = H_0^1(\Omega) \text{ and } N = \nabla, \text{ dom}(N) = H^1(\Omega) \quad (\text{A.8})$$

from  $L^2(\Omega; d^n x)$  to  $L^2(\Omega; d^n x)^n$  and note that

$$\tilde{H}_{0,\Omega}^D = D^* D \text{ and } \tilde{H}_{0,\Omega}^N = N^* N. \quad (\text{A.9})$$

For details we refer to [44, Sects. XIII.14, XIII.15]. Moreover, with  $\text{div}(\cdot)$  denoting the divergence operator,

$$\text{dom}(D^*) = \{w \in L^2(\Omega; d^n x)^n \mid \text{div}(w) \in L^2(\Omega; d^n x)\}, \quad (\text{A.10})$$

and hence,

$$\begin{aligned} \text{dom}(\tilde{H}_{0,\Omega}^D) &= \{u \in \text{dom}(D) \mid Du \in \text{dom}(D^*)\} \\ &= \{u \in H_0^1(\Omega) \mid \Delta u \in L^2(\Omega; d^n x)\}. \end{aligned} \quad (\text{A.11})$$

One can also define the following map

$$\begin{cases} \{w \in L^2(\Omega; d^n x)^n \mid \operatorname{div}(w) \in (H^1(\Omega))^*\} \rightarrow H^{-1/2}(\partial\Omega) = (H^{1/2}(\partial\Omega))^* \\ w \mapsto \nu \cdot w \end{cases} \quad (\text{A.12})$$

by setting

$$\langle \nu \cdot w, \phi \rangle = \int_{\Omega} d^n x w(x) \cdot \nabla \Phi(x) + \langle \operatorname{div}(w), \Phi \rangle \quad (\text{A.13})$$

whenever  $\phi \in H^{1/2}(\partial\Omega)$  and  $\Phi \in H^1(\Omega)$  is such that  $\gamma_D \Phi = \phi$ . The last pairing in (A.13) is in the duality sense (which, in turn, is compatible with the (bilinear) distributional pairing). It should be remarked that the above definition is independent of the particular extension  $\Phi \in H^1(\Omega)$  of  $\phi$ . Indeed, by linearity this comes down to proving that

$$\langle \operatorname{div}(w), \Phi \rangle = - \int_{\Omega} d^n x w(x) \cdot \nabla \Phi(x) \quad (\text{A.14})$$

if  $w \in L^2(\Omega; d^n x)^n$  has  $\operatorname{div}(w) \in (H^1(\Omega))^*$  and  $\Phi \in H^1(\Omega)$  has  $\gamma_D \Phi = 0$ . To see this, we rely on the existence of a sequence  $\Phi_j \in C_0^\infty(\Omega)$  such that  $\Phi_j \xrightarrow{j \uparrow \infty} \Phi$  in  $H^1(\Omega)$ .

When  $\Omega$  is a bounded Lipschitz domain, this is well-known (see, e.g., [22, Remark 2.7] for a rather general result of this nature), and this result is easily extended to the case when  $\Omega$  is an unbounded Lipschitz domain with a compact boundary. For if  $\xi \in C_0^\infty(B(0; 2))$  is such that  $\xi = 1$  on  $B(0; 1)$  and  $\xi_j(x) = \xi(x/j)$ ,  $j \in \mathbb{N}$  (here  $B(x_0; r_0)$  denotes the ball in  $\mathbb{R}^n$  centered at  $x_0 \in \mathbb{R}^n$  of radius  $r_0 > 0$ ), then  $\xi_j \Phi \xrightarrow{j \uparrow \infty} \Phi$  in  $H^1(\Omega)$  and matters are reduced to approximating  $\xi_j \Phi$  in  $H^1(B(0; 2j) \cap \Omega)$  with test functions supported in  $B(0; 2j) \cap \Omega$ , for each fixed  $j \in \mathbb{N}$ . Since  $\gamma_D(\xi_j \Phi) = 0$ , the result for bounded Lipschitz domains applies.

Returning to the task of proving (A.14), it suffices to prove a similar identity with  $\Phi_j$  in place of  $\Phi$ . This, in turn, follows from the definition of  $\operatorname{div}(\cdot)$  in the sense of distributions and the fact that the duality between  $(H^1(\Omega))^*$  and  $H^1(\Omega)$  is compatible with the duality between distributions and test functions.

Going further, we can introduce a (weak) Neumann trace operator  $\tilde{\gamma}_N$  as follows:

$$\tilde{\gamma}_N : \{u \in H^1(\Omega) \mid \Delta u \in (H^1(\Omega))^*\} \rightarrow H^{-1/2}(\partial\Omega), \quad \tilde{\gamma}_N u = \nu \cdot \nabla u, \quad (\text{A.15})$$

with the dot product understood in the sense of (A.12). We emphasize that the weak Neumann trace operator  $\tilde{\gamma}_N$  in (A.17) is an extension of the operator  $\gamma_N$  introduced in (6.43). Indeed, to see that  $\operatorname{dom}(\gamma_N) \subset \operatorname{dom}(\tilde{\gamma}_N)$ , we note that if  $u \in H^{s+1}(\Omega)$  for some  $1/2 < s < 3/2$ , then  $\Delta u \in H^{-1+s}(\Omega) = (H^{1-s}(\Omega))^* \hookrightarrow (H^1(\Omega))^*$ , by (A.5) and (A.4). With this in hand, it is then easy to show that  $\tilde{\gamma}_N$  in (A.17) and  $\gamma_N$  in (6.43) agree (on the smaller domain), as claimed.

We now return to the mainstream discussion. From the above preamble it follows that

$$\operatorname{dom}(N^*) = \{w \in L^2(\Omega; d^n x)^n \mid \operatorname{div}(w) \in L^2(\Omega; d^n x) \text{ and } \nu \cdot w = 0\} \quad (\text{A.16})$$

where the dot product operation is understood in the sense of (A.12). Consequently, with  $\tilde{H}_{0,\Omega}^N = N^*N$ , we have

$$\begin{aligned} \text{dom}(\tilde{H}_{0,\Omega}^N) &= \{u \in \text{dom}(N) \mid Nu \in \text{dom}(N^*)\} \\ &= \{u \in H^1(\Omega) \mid \Delta u \in L^2(\Omega; d^n x) \text{ and } \tilde{\gamma}_N u = 0\}. \end{aligned} \quad (\text{A.17})$$

Next, we will prove that  $H_{0,\Omega}^D = \tilde{H}_{0,\Omega}^D$  and  $H_{0,\Omega}^N = \tilde{H}_{0,\Omega}^N$ , where  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$  denote the operators introduced in (6.44) and (6.45), respectively. Since it follows from the first Green's formula (cf., e.g., [33, Theorem 4.4]) that  $H_{0,\Omega}^D \subseteq \tilde{H}_{0,\Omega}^D$  and  $H_{0,\Omega}^N \subseteq \tilde{H}_{0,\Omega}^N$ , it remains to show that  $H_{0,\Omega}^D \supseteq \tilde{H}_{0,\Omega}^D$  and  $H_{0,\Omega}^N \supseteq \tilde{H}_{0,\Omega}^N$ . Moreover, it follows from comparing (6.44) with (A.11) and (6.45) with (A.17), that one needs only to show that  $\text{dom}(\tilde{H}_{0,\Omega}^D), \text{dom}(\tilde{H}_{0,\Omega}^N) \subseteq H^2(\Omega)$ .

**Lemma A.1.** *Assume Hypothesis 6.6(i). Then,*

$$\text{dom}(H_{0,\Omega}^D) \subseteq H^2(\Omega), \quad \text{dom}(H_{0,\Omega}^N) \subseteq H^2(\Omega). \quad (\text{A.18})$$

*In particular,*

$$H_{0,\Omega}^D = \tilde{H}_{0,\Omega}^D, \quad H_{0,\Omega}^N = \tilde{H}_{0,\Omega}^N. \quad (\text{A.19})$$

*Proof.* Consider  $u \in \text{dom}(\tilde{H}_{0,\Omega}^N)$  and set  $f = \Delta u - u \in L^2(\Omega; d^n x)$ . Viewing  $f$  as an element in  $(H^1(\Omega))^*$ , the classical Lax-Milgram Lemma implies that  $u$  is the unique solution of the boundary-value problem

$$\begin{cases} (\Delta - I_\Omega)u = f \in L^2(\Omega) \hookrightarrow (H^1(\Omega))^*, \\ u \in H^1(\Omega), \\ \tilde{\gamma}_N u = 0. \end{cases} \quad (\text{A.20})$$

One convenient way to show that actually

$$u \in H^2(\Omega), \quad (\text{A.21})$$

is to use layer potentials. Specifically, let  $E(x)$ ,  $x \in \mathbb{R}^n \setminus \{0\}$ , be the fundamental solution of the Helmholtz operator  $\Delta - I_\Omega$  in  $\mathbb{R}^n$  and denote by  $(\Delta - I_\Omega)^{-1}$  the operator of convolution with  $E$ . Let us also define the associated single layer potential

$$\mathcal{S}g(x) = \int_{\partial\Omega} d^{n-1}\sigma_y E(x-y)g(y), \quad x \in \Omega, \quad (\text{A.22})$$

where  $g$  is an arbitrary measurable function on  $\partial\Omega$ . As is well-known (the interested reader may consult, e.g., [34], [60] for jump relations in the context of Lipschitz domains), if

$$K^\#g(x) = \int_{\partial\Omega} d^{n-1}\sigma_y \partial_{\nu_x} E(x-y)g(y), \quad x \in \partial\Omega \quad (\text{A.23})$$

stands for the so-called adjoint double layer on  $\partial\Omega$ , the following jump formula holds

$$\tilde{\gamma}_N \mathcal{S}g = (\tfrac{1}{2}I_{\partial\Omega} + K^\#)g. \quad (\text{A.24})$$

Now, the solution  $u$  of (A.20) is given by

$$u = (\Delta - I_\Omega)^{-1}f - \mathcal{S}g \quad (\text{A.25})$$

for a suitable chosen  $g$ . In order to continue, we recall that the classical Calderón-Zygmund theory yields that, locally,  $(\Delta - I_\Omega)^{-1}$  is smoothing of order 2 on the



scale of Sobolev spaces, and since  $E$  has exponential decay at infinity, it follows that  $(\Delta - I_\Omega)^{-1}f \in H^2(\Omega)$  whenever  $f \in L^2(\Omega; d^n x)$ . We shall then require that

$$\gamma_N \mathcal{S}g = \gamma_N(\Delta - I_\Omega)^{-1}f \text{ or } (\tfrac{1}{2}I_{\partial\Omega} + K^\#)g = h = \gamma_N(\Delta - I_\Omega)^{-1}f \in H^{1/2}(\partial\Omega). \quad (\text{A.26})$$

Thus, formally,  $g = (\tfrac{1}{2}I_{\partial\Omega} + K^\#)^{-1}h$  and (A.21) follows as soon as we prove that

$$\tfrac{1}{2}I_{\partial\Omega} + K^\# \text{ is invertible on } H^{1/2}(\partial\Omega) \quad (\text{A.27})$$

and that the operator

$$\mathcal{S}: H^{1/2}(\partial\Omega) \rightarrow H^2(\partial\Omega) \quad (\text{A.28})$$

is well-defined and bounded. That (A.27) holds is essentially well-known. See, for instance, [57, Proposition 4.5] which requires that  $\Omega$  is of class  $C^{1,r}$  for some  $(1/2) < r < 1$ . As for (A.28), we note, as a preliminary step, that

$$\mathcal{S}: H^{-s}(\partial\Omega) \rightarrow H^{-s+3/2}(\Omega) \quad (\text{A.29})$$

is well-defined and bounded for each  $s \in [0, 1]$ , even when the boundary of  $\Omega$  is only Lipschitz. Indeed, with  $H^{-s+3/2}(\Omega)$  replaced by  $H^{-s+3/2}(\Omega \cap B)$  for a sufficiently large ball  $B \subset \mathbb{R}^n$ , this is proved in [35] and the behavior at infinity is easily taken care of by employing the exponential decay of  $E$ .

For a fixed, arbitrary  $j \in \{1, \dots, n\}$ , consider next the operator  $\partial_{x_j} \mathcal{S}$  whose kernel is  $\partial_{x_j} E(x - y) = -\partial_{y_j} E(x - y)$ . We write

$$\partial_{y_j} = \sum_{k=1}^n \nu_k(y) \nu_k(y) \partial_{y_j} = \sum_{k=1}^n \nu_k(y) \frac{\partial}{\partial \tau_{k,j}(y)} + \nu_j \partial_{\nu_j}, \quad (\text{A.30})$$

where  $\partial/\partial \tau_{k,j} = \nu_k \partial_j - \nu_j \partial_k$ ,  $j, k = 1, \dots, n$ , is a tangential derivative operator for which we have

$$\int_{\partial\Omega} d^{n-1} \sigma \frac{\partial h_1}{\partial \tau_{j,k}} h_2 = - \int_{\partial\Omega} d^{n-1} \sigma h_1 \frac{\partial h_2}{\partial \tau_{j,k}}, \quad h_1, h_2 \in H^{1/2}(\partial\Omega). \quad (\text{A.31})$$

It follows that

$$\partial_j \mathcal{S}h = -\mathcal{D}(\nu_j h) + \sum_{k=1}^n \mathcal{S} \left( \frac{\partial(\nu_k h)}{\partial \tau_{k,j}} \right), \quad (\text{A.32})$$

where  $\mathcal{D}$ , the so-called double layer potential operator, is the integral operator with integral kernel  $\partial_{\nu_y} E(x - y)$ . Its mappings properties on the scale of Sobolev spaces have been analyzed in [35] and we note here that

$$\mathcal{D}: H^s(\partial\Omega) \rightarrow H^{s+1/2}(\Omega), \quad 0 \leq s \leq 1, \quad (\text{A.33})$$

requires only that  $\partial\Omega$  is Lipschitz.

Assuming that multiplication by (the components of)  $\nu$  preserves the space  $H^{1/2}(\partial\Omega)$  (which is the case if, e.g.,  $\Omega$  is of class  $C^{1,r}$  for some  $(1/2) < r < 1$ ), the desired conclusion about the operator (A.28) follows from (A.29), (A.32) and (A.33). This concludes the proof of the fact that  $\text{dom}(H_{0,\Omega}^N) \subseteq H^2(\Omega)$ .

To prove that  $\text{dom}(H_{0,\Omega}^D) \subseteq H^2(\Omega)$  we proceed in an analogous fashion, starting with the same representation (A.25). This time, the requirement on  $g$  is that  $\mathcal{S}g = h = \gamma_D(\Delta - I_\Omega)^{-1}f \in H^{3/2}(\partial\Omega)$ , where  $S = \gamma_D \circ \mathcal{S}$  is the trace of the single layer. Thus, in this scenario, it suffices to know that

$$S: H^{1/2}(\partial\Omega) \rightarrow H^{3/2}(\partial\Omega) \quad (\text{A.34})$$

is an isomorphism. When  $\partial\Omega$  is of class  $C^\infty$ , it has been proved in [57, Proposition 7.9] that  $S: H^s(\partial\Omega) \rightarrow H^{s+1}(\partial\Omega)$  is an isomorphism for each  $s \in \mathbb{R}$  and, if  $\Omega$  is of class  $C^{1,r}$  with  $(1/2) < r < 1$ , the validity range of this result is limited to  $-1 - r < s < r$ , which covers (A.34). The latter fact follows from an inspection of Taylor's original proof of Proposition 7.9 in [57]. Here we just note that the only significant difference is that if  $\partial\Omega$  is of class  $C^{1,r}$  (instead of class  $C^\infty$ ), then  $S$  is a pseudodifferential operator whose symbol exhibits a limited amount of regularity in the space-variable. Such classes of operators have been studied in, e.g., [34], [56, Chs. 1, 2].  $\square$

We note that Lemma A.1 also follows from [10, Theorem 8.2] in the case of  $C^2$ -domains  $\Omega$  with compact boundary. This is proved in [10] by rather different methods and can be viewed as a generalization of the classical result for bounded  $C^2$ -domains.

**Lemma A.2.** *Assume Hypothesis 6.6(i) and let  $q \in \mathbb{R}$ . Then for each  $z \in \mathbb{C} \setminus [0, \infty)$ , one has*

$$(H_{0,\Omega}^D - zI_\Omega)^{-q}, (H_{0,\Omega}^N - zI_\Omega)^{-q} \in \mathcal{B}(L^2(\Omega; d^n x), H^{2q}(\Omega)). \quad (\text{A.35})$$

*Proof.* For notational convenience, we denote by  $H_{0,\Omega}$  either one of the operators  $H_{0,\Omega}^D$  or  $H_{0,\Omega}^N$ . The operator  $H_{0,\Omega}$  is a semibounded self-adjoint operator in  $L^2(\Omega; d^n x)$ , and thus the resolvent set of  $H_{0,\Omega}$  is linearly connected.

Step 1: We claim that it is enough to prove (A.35) for one point  $z$  in the resolvent set of  $H_{0,\Omega}$ . Indeed, suppose that (A.35) holds, and  $z'$  is any other point in the resolvent set of  $H_{0,\Omega}$ . Connecting  $z$  and  $z'$  by a curve in the resolvent set, and splitting this curve in small segments, without loss of generality we may assume that  $z'$  is arbitrarily close to  $z$  so that the operator  $I_\Omega - (z' - z)(H_{0,\Omega} - zI_\Omega)^{-1}$  is invertible, and thus the operator  $(I_\Omega - (z' - z)(H_{0,\Omega} - zI_\Omega)^{-1})^{-q}$  is a bounded operator on  $L^2(\Omega; d^n x)$ . Then (A.35) and the identity

$$(H_{0,\Omega} - z'I_\Omega)^{-q} = (H_{0,\Omega} - zI_\Omega)^{-q} (I_\Omega - (z' - z)(H_{0,\Omega} - zI_\Omega)^{-1})^{-q} \quad (\text{A.36})$$

imply (A.35) with  $z$  replaced by  $z'$ , proving the claim.

Step 2: By [33, Theorem B.8] (cf. also Theorem 4.3.1.2 and Remark 4.3.1.2 in [58]), if  $\Omega \subseteq \mathbb{R}^n$  is a Lipschitz domain,  $n \in \mathbb{N}$ , and  $s_0, s_1 \in \mathbb{R}$ , then

$$\left( H^{s_0}(\Omega), H^{s_1}(\Omega) \right)_{\theta, 2} = H^s(\Omega), \quad s = (1 - \theta)s_0 + \theta s_1, \quad 0 < \theta < 1. \quad (\text{A.37})$$

Here, for Banach spaces  $\mathcal{X}_0$  and  $\mathcal{X}_1$ , we denote by  $(\mathcal{X}_0, \mathcal{X}_1)_{\theta, p}$  the real interpolation space (obtained by the  $K$ -method), as discussed, for instance, in [33, Appendix B] and [58, Sect. 1.3]. Letting  $s_0 = 0$ ,  $s_1 = 2$ , and  $s = 2q$ , one then infers

$$\left( L^2(\Omega; d^n x), H^2(\Omega) \right)_{q, 2} = H^{2q}(\Omega). \quad (\text{A.38})$$

Step 3: Using the claim in Step 1, we may assume without loss of generality that  $H_{0,\Omega} - zI_\Omega$  is a strictly positive operator and thus the fractional power  $(H_{0,\Omega} - zI_\Omega)^q$  can be defined via its spectral decomposition (see, e.g., [58, Sec.1.18.10]). We remark that the operator  $(H_{0,\Omega} - zI_\Omega)^q$  is an isomorphism between the Banach space  $\text{dom}(H_{0,\Omega} - zI_\Omega)^q$ , equipped with the graph-norm, and the space  $L^2(\Omega; d^n x)$ , and thus

$$(H_{0,\Omega} - zI_\Omega)^{-q} \in \mathcal{B}(L^2(\Omega; d^n x), \text{dom}((H_{0,\Omega} - zI_\Omega)^q)). \quad (\text{A.39})$$

By an abstract interpolation result for strictly positive, self-adjoint operators, see [58, Theorem 1.18.10], for any  $\alpha, \beta \in \mathbb{C}$  with  $\operatorname{Re} \alpha, \operatorname{Re} \beta \geq 0$  and  $\theta \in (0, 1)$  one has,

$$\left( \operatorname{dom}((H_{0,\Omega} - zI_\Omega)^\alpha), \operatorname{dom}((H_{0,\Omega} - zI_\Omega)^\beta) \right)_{\theta,2} = \operatorname{dom}((H_{0,\Omega} - zI_\Omega)^{\alpha(1-\theta)+\beta\theta}). \quad (\text{A.40})$$

Applying this result with  $\alpha = 0$  and  $\beta = 1$ , one infers

$$\left( L^2(\Omega; d^n x), \operatorname{dom}(H_{0,\Omega} - zI_\Omega) \right)_{q,2} = \operatorname{dom}((H_{0,\Omega} - zI_\Omega)^q). \quad (\text{A.41})$$

Noting that  $\operatorname{dom}(H_{0,\Omega}) = \operatorname{dom}(H_{0,\Omega} - zI_\Omega)$ , and using (A.38), (A.41), and Lemma A.1, one arrives at the continuous imbedding

$$\operatorname{dom}((H_{0,\Omega} - zI_\Omega)^q) \hookrightarrow H^{2q}(\Omega). \quad (\text{A.42})$$

Thus, (A.35) is a consequence of (A.39) and (A.42).  $\square$

Finally, we will prove an extension of a result of Nakamura [36, Lemma 6] from a cube in  $\mathbb{R}^n$  to a Lipschitz domain  $\Omega$ . This requires some preparations. First, we note that (A.15) and (A.13) yield the following Green formula

$$\langle \tilde{\gamma}_N u, \gamma_D \Phi \rangle = (\overline{\nabla u}, \nabla \Phi)_{L^2(\Omega; d^n x)^n} + \langle \Delta u, \Phi \rangle, \quad (\text{A.43})$$

valid for any  $u \in H^1(\Omega)$  with  $\Delta u \in (H^1(\Omega))^*$ , and any  $\Phi \in H^1(\Omega)$ . The pairing on the left-hand side of (A.43) is between functionals in  $(H^{1/2}(\partial\Omega))^*$  and elements in  $H^{1/2}(\partial\Omega)$ , whereas the last pairing on the right-hand side is between functionals in  $(H^1(\Omega))^*$  and elements in  $H^1(\Omega)$ . For further use, we also note that the adjoint of (6.42) maps as follows

$$\gamma_D^* : (H^{s-1/2}(\partial\Omega))^* \rightarrow (H^s(\Omega))^*, \quad 1/2 < s < 3/2. \quad (\text{A.44})$$

Next we observe that the operator  $(\tilde{H}_{0,\Omega}^N - zI_\Omega)^{-1}$ ,  $z \in \mathbb{C} \setminus \sigma(\tilde{H}_{0,\Omega}^N)$ , originally defined as

$$(\tilde{H}_{0,\Omega}^N - zI_\Omega)^{-1} : L^2(\Omega; d^n x) \rightarrow L^2(\Omega; d^n x), \quad (\text{A.45})$$

can be extended to a bounded operator, mapping  $(H^1(\Omega))^*$  into  $L^2(\Omega; d^n x)$ . Specifically, since  $(\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} : L^2(\Omega; d^n x) \rightarrow \operatorname{dom}(\tilde{H}_{0,\Omega}^N)$  is bounded and since the inclusion  $\operatorname{dom}(\tilde{H}_{0,\Omega}^N) \hookrightarrow H^1(\Omega)$  is bounded, we can naturally view  $(\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}$  as an operator

$$(\hat{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1} : L^2(\Omega; d^n x) \rightarrow H^1(\Omega) \quad (\text{A.46})$$

mapping in a linear, bounded fashion. Consequently, for its adjoint, we have

$$((\hat{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1})^* : (H^1(\Omega))^* \rightarrow L^2(\Omega; d^n x), \quad (\text{A.47})$$

and it is easy to see that this latter operator extends the one in (A.45). Hence, there is no ambiguity in retaining the same symbol, that is,  $(\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}$ , both for the operator in (A.47) as well as for the operator in (A.45). Similar considerations and conventions apply to  $(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}$ .

**Lemma A.3.** *Let  $\Omega \subset \mathbb{R}^n$ ,  $n \geq 2$ , be a Lipschitz domain and let  $z \in \mathbb{C} \setminus (\sigma(\tilde{H}_{0,\Omega}^D) \cup \sigma(\tilde{H}_{0,\Omega}^N))$ . Then, on  $L^2(\Omega; d^n x)$ ,*

$$(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1} - (\tilde{H}_{0,\Omega}^N - zI_\Omega)^{-1} = (\tilde{H}_{0,\Omega}^N - zI_\Omega)^{-1} \gamma_D^* \tilde{\gamma}_N (\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}, \quad (\text{A.48})$$

where  $\gamma_D^*$  is an adjoint operator to  $\gamma_D$  in the sense of (A.44)

*Proof.* To set the stage, we note that the composition of operators appearing on the right-hand side of (A.48) is meaningful since

$$(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}: L^2(\Omega; d^n x) \rightarrow \text{dom}(\tilde{H}_{0,\Omega}^D) \subset \{u \in H^1(\Omega) \mid \Delta u \in (H^1(\Omega))^*\}, \quad (\text{A.49})$$

$$\tilde{\gamma}_N: \{u \in H^1(\Omega) \mid \Delta u \in (H^1(\Omega))^*\} \rightarrow H^{-1/2}(\partial\Omega) \quad (\text{A.50})$$

$$\gamma_D^*: (H^{1/2}(\partial\Omega))^* = H^{-1/2}(\partial\Omega) \rightarrow (H^1(\Omega))^*, \quad (\text{A.51})$$

$$(\tilde{H}_{0,\Omega}^N - zI_\Omega)^{-1}: (H^1(\Omega))^* \rightarrow L^2(\Omega; d^n x), \quad (\text{A.52})$$

with the convention made just before the statement of the lemma used in the last line. Next, let  $\phi_1, \psi_1 \in L^2(\Omega; d^n x)$  be arbitrary and define

$$\begin{aligned} \phi &= (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\phi_1 \in \text{dom}(\tilde{H}_{0,\Omega}^N) \subset H^1(\Omega), \\ \psi &= (\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1 \in \text{dom}(\tilde{H}_{0,\Omega}^D) \subset H^1(\Omega). \end{aligned} \quad (\text{A.53})$$

It therefore suffices to show that the following identity holds:

$$\begin{aligned} &(\phi_1, (\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)} - (\phi_1, (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)} \\ &= (\phi_1, (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\gamma_D^*\tilde{\gamma}_N(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)}. \end{aligned} \quad (\text{A.54})$$

We note that according to (A.53) one has,

$$(\phi_1, (\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)} = ((\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)\phi, \psi)_{L^2(\Omega; d^n x)}, \quad (\text{A.55})$$

$$\begin{aligned} (\phi_1, (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)} &= (((\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1})^*\phi_1, \psi_1)_{L^2(\Omega; d^n x)} \\ &= ((\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\phi_1, \psi_1)_{L^2(\Omega; d^n x)} \\ &= (\phi, (\tilde{H}_{0,\Omega}^D - zI_\Omega)\psi)_{L^2(\Omega; d^n x)}, \end{aligned} \quad (\text{A.56})$$

and, keeping in mind the convention adopted prior to the statement of the lemma,

$$\begin{aligned} &(\phi_1, (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\gamma_D^*\tilde{\gamma}_N(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1)_{L^2(\Omega; d^n x)} \\ &= \overline{\langle (\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\phi_1, \gamma_D^*\tilde{\gamma}_N(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1 \rangle} \\ &= \langle \gamma_D(\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}\phi_1, \tilde{\gamma}_N(\tilde{H}_{0,\Omega}^D - zI_\Omega)^{-1}\psi_1 \rangle = \langle \overline{\gamma_D\phi}, \tilde{\gamma}_N\psi \rangle \end{aligned} \quad (\text{A.57})$$

where  $\langle \cdot, \cdot \rangle$  stands for pairings between Sobolev spaces (in  $\Omega$  and  $\partial\Omega$ ) and their duals. Thus, matters have been reduced to proving that

$$((\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)\phi, \psi)_{L^2(\Omega; d^n x)} - (\phi, (\tilde{H}_{0,\Omega}^D - zI_\Omega)\psi)_{L^2(\Omega; d^n x)} = \langle \overline{\gamma_D\phi}, \tilde{\gamma}_N\psi \rangle. \quad (\text{A.58})$$

Using (A.43) for the left-hand side of (A.58) one obtains

$$\begin{aligned} &((\tilde{H}_{0,\Omega}^N - \bar{z}I_\Omega)\phi, \psi)_{L^2(\Omega; d^n x)} - (\phi, (\tilde{H}_{0,\Omega}^D - zI_\Omega)\psi)_{L^2(\Omega; d^n x)} \\ &= -(\Delta\phi, \psi)_{L^2(\Omega; d^n x)} + (\phi, \Delta\psi)_{L^2(\Omega; d^n x)} \\ &= (\nabla\phi, \nabla\psi)_{L^2(\Omega; d^n x)} - \langle \overline{\tilde{\gamma}_N\phi}, \gamma_D\psi \rangle - (\nabla\phi, \nabla\psi)_{L^2(\Omega; d^n x)} + \langle \overline{\gamma_D\phi}, \tilde{\gamma}_N\psi \rangle \\ &= -\langle \overline{\tilde{\gamma}_N\phi}, \gamma_D\psi \rangle + \langle \overline{\gamma_D\phi}, \tilde{\gamma}_N\psi \rangle. \end{aligned} \quad (\text{A.59})$$

Observing that  $\tilde{\gamma}_N\phi = 0$  since  $\phi \in \text{dom}(H_{0,\Omega}^N)$ , one concludes (A.58).  $\square$

**Remark A.4.** While it is tempting to view  $\gamma_D$  as an unbounded but densely defined operator on  $L^2(\Omega; d^n x)$  whose domain contains the space  $C_0^\infty(\Omega)$ , one should note that in this case its adjoint  $\gamma_D^*$  is not densely defined: Indeed, the adjoint  $\gamma_D^*$  of  $\gamma_D$  would have to be an unbounded operator from  $L^2(\partial\Omega; d^{n-1}\sigma)$  to  $L^2(\Omega; d^n x)$  such that

$$(\gamma_D f, g)_{L^2(\partial\Omega; d^{n-1}\sigma)} = (f, \gamma_D^* g)_{L^2(\Omega; d^n x)} \quad \text{for all } f \in \text{dom}(\gamma_D), g \in \text{dom}(\gamma_D^*). \quad (\text{A.60})$$

In particular, choosing  $f \in C_0^\infty(\Omega)$ , in which case  $\gamma_D f = 0$ , one concludes that  $(f, \gamma_D^* g)_{L^2(\Omega; d^n x)} = 0$  for all  $f \in C_0^\infty(\Omega)$ . Thus, one obtains  $\gamma_D^* g = 0$  for all  $g \in \text{dom}(\gamma_D^*)$ . Since obviously  $\gamma_D \neq 0$ , (A.60) implies  $\text{dom}(\gamma_D^*) = \{0\}$  and hence  $\gamma_D$  is not a closable linear operator in  $L^2(\Omega; d^n x)$ .

**Remark A.5.** In the case of a domain  $\Omega$  of class  $C^{1,r}$ ,  $(1/2) < r < 1$ , the operators  $\tilde{H}_{0,\Omega}^D$  and  $\tilde{H}_{0,\Omega}^N$  coincide with the operators  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$ , respectively, and hence one can use the operators  $H_{0,\Omega}^D$  and  $H_{0,\Omega}^N$  in Lemma A.3. Moreover, since  $\text{dom}(H_{0,\Omega}^D) \subseteq H^2(\Omega)$ , one can also replace  $\tilde{\gamma}_N$  by  $\gamma_N$  (cf. (6.43)) in Lemma A.3. In particular,

$$(H_{0,\Omega}^D - zI_\Omega)^{-1} - (H_{0,\Omega}^N - zI_\Omega)^{-1} = [\gamma_D(H_{0,\Omega}^N - \bar{z}I_\Omega)^{-1}]^* \gamma_N(H_{0,\Omega}^D - zI_\Omega)^{-1}. \quad (\text{A.61})$$

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